

### From the INTERNATIONAL BUREAU

# To: PCT United States Patent and Trademark NOTIFICATION OF ELECTION Office (Box PCT) (PCT Rule 61.2) Crystal Plaza 2 Washington, DC 20231 ÉTATS-UNIS D'AMÉRIQUE Date of mailing: in its capacity as elected Office 08 July 1999 (08.07.99) Applicant's or agent's file reference: International application No.: PP/2560 PCT PCT/GB98/03860 Priority date: International filing date: 24 December 1997 (24.12.97) 24 December 1998 (24.12.98) Applicant: SCHOFIELD, Christopher, Joseph et al 1. The designated Office is hereby notified of its election made: in the demand filed with the International preliminary Examining Authority on: 06 May 1999 (06.05.99) in a notice effecting later election filed with the International Bureau on: 2. The election was not made before the expiration of 19 months from the priority date or, where Rule 32 applies, within the time limit under Rule 32.2(b).

The International Bureau of WIPO 34, chemin des Colombettes 1211 Geneva 20, Switzerland Authorized officer:

Facsimile No.: (41-22) 740.14.35

J. Zahra Telephone No.: (41-22) 338.83.38

# PATENT COOPERATION TREATY

	From the	INTERNATIONAL BUI	REAU
PCT To:			
OF A CHANGE Steve 1 Ser (PCT Rule 92bis.1 and Administrative Instructions, Section 422) Lond ROY		NANT, Pyers ens Hewlett & Perkins rjeants' Inn Street Ion, Greater London EC4Y 1LL AUME-UNI	
Date of mailing (day/month/year) 02 May 2000 (02.05.00)			
Applicant's or agent's file reference PP/2560 PCT		IMPORTANT NOTIF	
International application No. PCT/GB98/03860		al filing date (day/month/yea ecember 1998 (24.12.96	
The following indications appeared on record concerning:      The following indications appeared on record concerning:     The following indications appeared on record concerning:     The following indications appeared on record concerning:	the agen		n representative
Name and Address ISIS INNOVATION LIMITED 2 South Parks Road Oxford OxfordOxfordShire OX1 3UB		State of Nationality GB Telephone No.	GB
United Kingdom		Facsimile No. Teleprinter No.	
The International Bureau hereby notifies the applicant that to the person     the name     X the adventional Bureau hereby notifies the applicant that to the person	he following	change has been recorded of the nationality	concerning: the residence
Name and Address		State of Nationality  GB	State of Residence GB
ISIS INNOVATION LIMITED  Ewer House Ewert Place Summertown		Telephone No.	
Oxford OX2 7BZ United Kingdom		Facsimile No.	
		Teleprinter No.	
3. Further observations, if necessary:			
4. A copy of this notification has been sent to:			
X the receiving Office the International Searching Authority		the designated Offices concerned  X the elected Offices concerned	
the International Preliminary Examining Authority		other:	
		rized officer  1. Britel	
		phone No.: (41-22) 338.83.38	

# PATENT COOPERATION TREATY

From the INTERNATIONAL BUREAU

### NOTIFICATION OF THE RECORDING **OF A CHANGE**

PENNANT, Pyers Stevens Hewlett & Perkins

(PCT Rule 92bis.1 and Administrative Instructions, Section 422)	Halton House 20/23 Holborn London EC1N 2JD ROYAUME-UNI
Date of mailing (day/month/year) 09 May 2000 (09.05.00)	
Applicant's or agent's file reference PP/2560 PCT	IMPORTANT NOTIFICATION
International application No. PCT/GB98/03860	International filing date (day/month/year) 24 December 1998 (24.12.98)
The following indications appeared on record concerning:     the applicant the inventor	the agent the common representative    State of Nationality   State of Residence
Name and Address	State of Nationality State of Residence
PENNANT, Pyers Stevens Hewlett & Perkins 1 Serjeants' Inn	Telephone No.
Fleet Street	44 171 936 2499
London, Greater London EC4Y 1LL United Kingdom	Facsimile No. 44 171 936 2498
	Teleprinter No.
2. The International Bureau hereby notifies the applicant that t	the following change has been recorded concerning:
the person the name X the ad	dress the nationality the residence
Name and Address	State of Nationality State of Residence
PFNNANT, Pvers	
Stevens Hewlett & Perkins Halton House	Telephone No. 44 20 7404 1955
20/23 Holborn London EC1N 2JD United Kingdom	Facsimile No.
Office Kingdom	44 20 7404 1844
	Teleprinter No.
3. Further observations, if necessary:	
4. A copy of this notification has been sent to:	
네네프(M) 사용하다면서 성향수를 받는 경기 전환 시간 ()	the designated Offices concerned
X the receiving Office the International Searching Authority	X the elected Offices concerned
the International Preliminary Examining Authority	other:
The International Bureau of WIPO	Authorized officer

34, chemin des Colombettes 1211 Geneva 20, Switzerland

Telephone No.: (41-22) 338.83.38

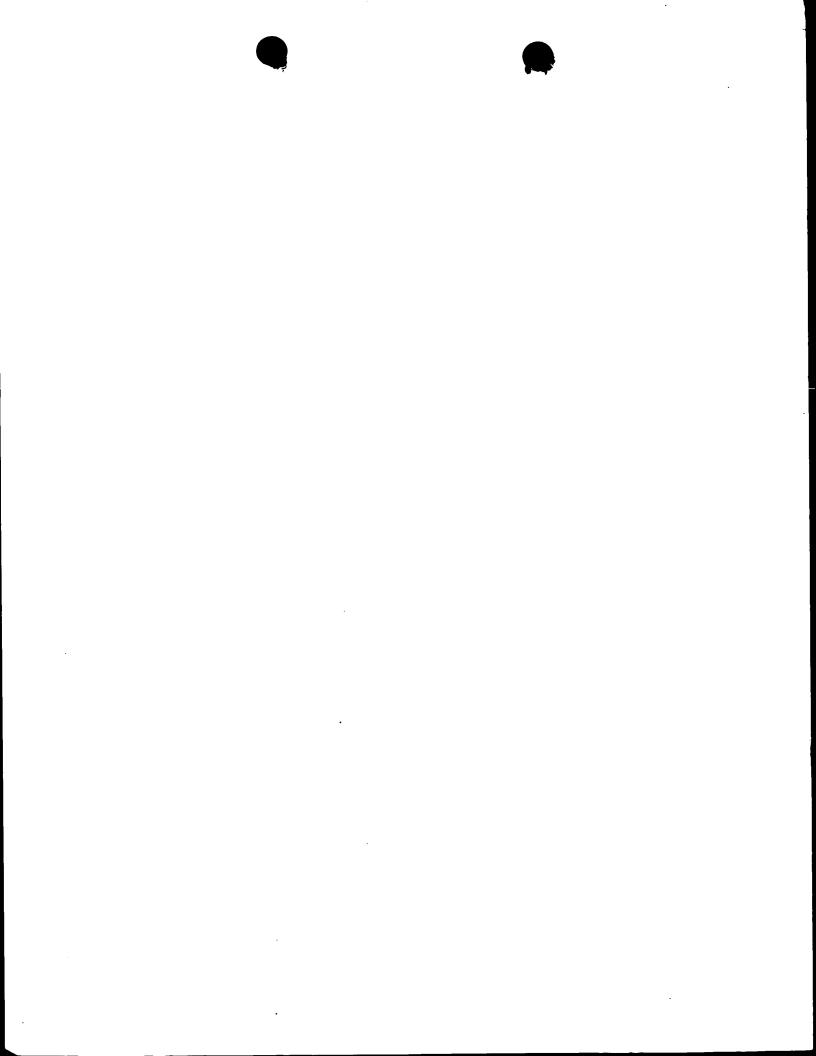
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### INTERNATIONAL SEARCH REPORT

(PCT Article 18 and Rules 43 and 44)

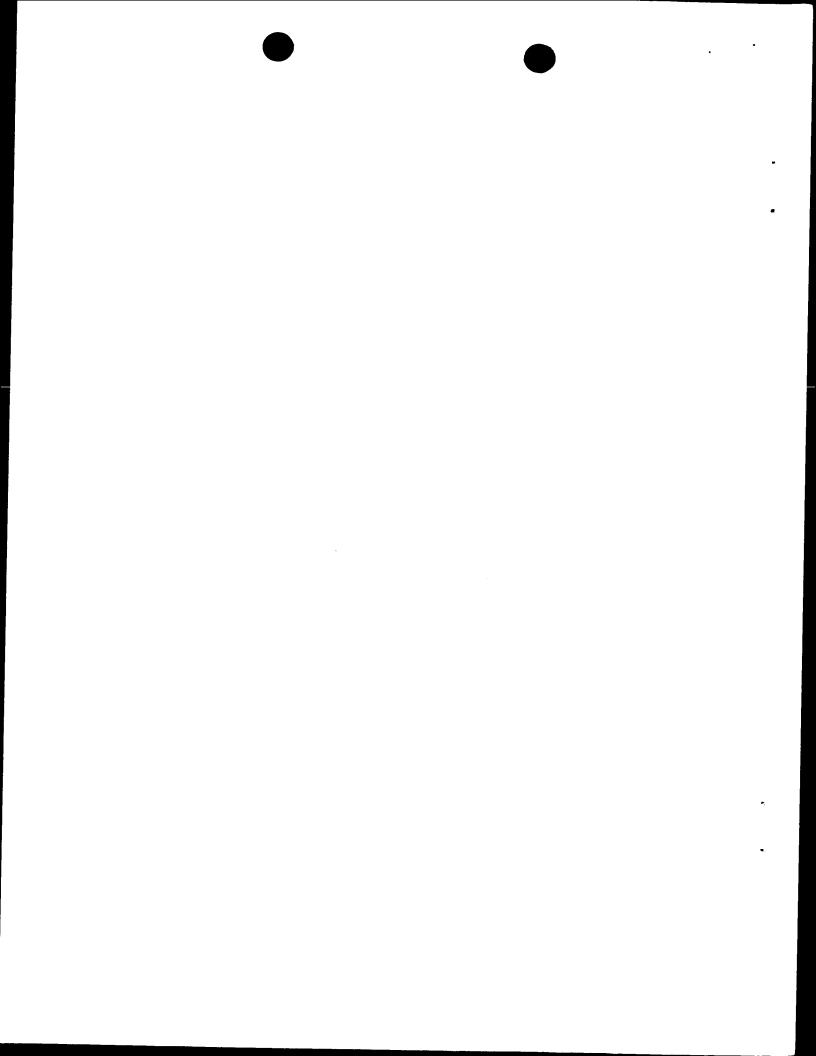
Applicant's or agent's file reference	FOR FURTHER see Notification of Transmittal of International Search Report			
PP/2560 PCT	ACTION (Form PCT/ISA/220) as well as, where applicable, item 5 below.			
International application No.	International filing date (day/month/year)	(Earliest) Priority Date (day/month/year)		
PCT/GB 98/03860	24/12/1998	24/12/1997		
Applicant				
ISIS INNOVATION LIMITED et	t al.			
-				
This International Search Report has been according to Article 18. A copy is being tra	n prepared by this International Searching Auth	ority and is transmitted to the applicant		
,	in Direction and International Bureau.			
This International Search Report consists				
It is also accompanied by	a copy of each prior art document cited in this	report.		
Basis of the report				
a. With regard to the language, the in	nternational search was carried out on the bas	is of the international application in the		
language in which it was filed, unle	ess otherwise indicated under this item.			
the international search was Authority (Rule 23.1(b)).	as carried out on the basis of a translation of th	e international application furnished to this		
b. With regard to any nucleotide and	d/or amino acid sequence disclosed in the int	ernational application, the international search		
was carried out on the basis of the	sequence listing : nal application in written form.			
<del>_</del>	national application in computer readable form			
	this Authority in written form.			
furnished subsequently to	this Authority in computer readble form.			
the statement that the subs international application as	sequently furnished written sequence listing do filed has been furnished.	es not go beyond the disclosure in the		
		identical to the written sequence listing has been		
2. Certain claims were foun	d unsearchable (See Box I).			
3. Unity of invention is lack				
4. With regard to the title,				
the text is approved as sub  the text has been establish				
	ed by this Authority to read as follows: ALOSPORIN C SYNTHASE (DAOCS	) AND Y_DAY STRUCTURE		
)	TEGOTORIN O STRINASE (DAGES	AND A RAI STRUCTURE		
5. With regard to the abstract,				
the text is approved as sub				
the text has been established within one month from the control	ed, according to Rule 38.2(b), by this Authority date of mailing of this international search repo	as it appears in Box III. The applicant may, rt, submit comments to this Authority.		
6. The figure of the <b>drawings</b> to be publis		<u></u>		
as suggested by the applica		None of the figures.		
because the applicant failed	d to suggest a figure.	-		
because this figure better c	haracterizes the invention.			



A. CLASSIFICATION OF SUBJECT MATTER IPC 6 C12N15/52 C12N C12P35/00 C12N9/00 According to International Patent Classification (IPC) or to both national classification and IPC **B. FIELDS SEARCHED** Minimum documentation searched (classification system followed by classification symbols) C12N C12P IPC 6 Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched Electronic data base consulted during the international search (name of data base and, where practical, search terms used) C. DOCUMENTS CONSIDERED TO BE RELEVANT Relevant to claim No. Citation of document, with indication, where appropriate, of the relevant passages Category 3 CORTES, JESUS ET AL: "Purification and 1 Χ characterization of a 2-oxoglutarate-linked ATP-independent deacetoxycephalosporin C synthase of Streptomyces lactamdurans" J. GEN. MICROBIOL. (1987), 133(11), 3165-74 CODEN: JGMIAN; ISSN: 0022-1287, 1987, XP000035085 2,3, see the whole document Y 21 - 26Patent family members are listed in annex. Further documents are listed in the continuation of box C. Special categories of cited documents: "T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the "A" document defining the general state of the art which is not considered to be of particular relevance invention "E" earlier document but published on or after the international "X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone filing date "L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified) "Y" document of particular relevance; the claimed invention cannot be considered to involve an invention step when the document is combined with one or more other such docu-"O" document referring to an oral disclosure, use, exhibition or ments, such combination being obvious to a person skilled other means in the art. document published prior to the international filing date but later than the pnority date claimed "&" document member of the same patent family Date of mailing of the international search report Date of the actual completion of the international search 26/03/1999 15 March 1999 Authorized officer Name and mailing address of the ISA European Patent Office, P.B. 5818 Patentiaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016

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Hix, R

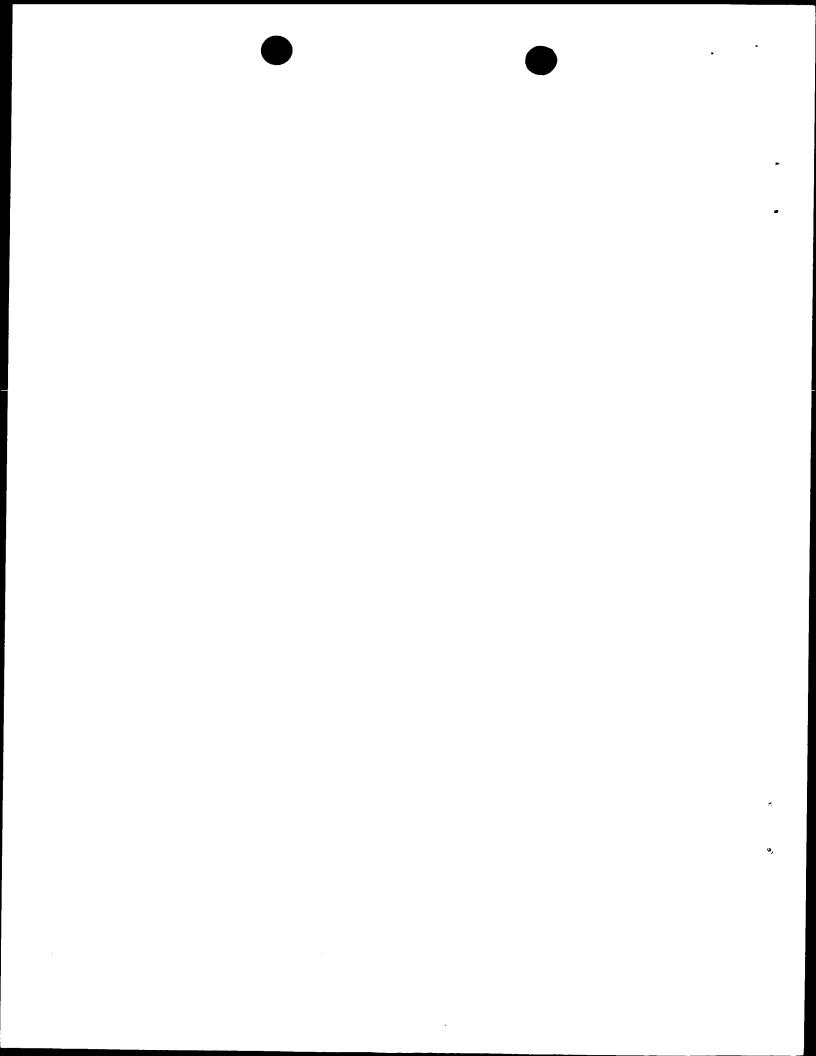


# INTERNATIONAL SEARCH REPORT

Int. Inchair Application No PCT/GB 98/03860

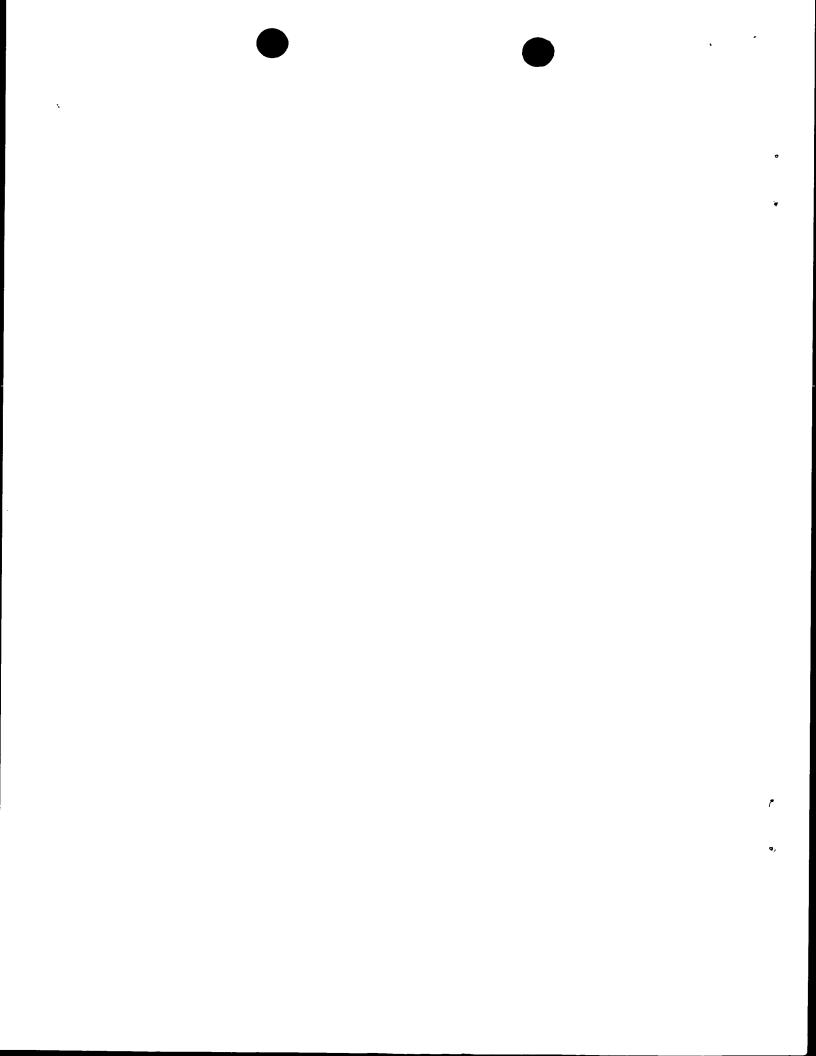
C.(Continua	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	
Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
*	ROLLINS, M. J. ET AL: "Purification and initial characterization of deacetoxycephalosporin C synthase from Streptomyces clavuligerus" CAN. J. MICROBIOL. (1988), 34(11), 1196-202 CODEN: CJMIAZ;ISSN: 0008-4166, 1988, XP002095821	1
Υ	see the whole document	2,3, 21-26
<i>y</i>	ROLLINS M J ET AL: "ISOPENICILLIN N SYNTHASE AND DEACETOXYCEPHALOSPORIN C SYNTHASE ACTIVITIES DURING DEFINED MEDIUM FERMENTATIONS OF STREPTOMYCES-CLAVULIGERUS EFFECT OF OXYGEN AND IRON SUPPLEMENTS" CAN J MICROBIOL, (1989) 35 (12), 1111-1117. CODEN: CJMIAZ. ISSN: 0008-4166., XP002095822	1
Y	see the whole document	2,3, 21-26
Ж	DOTZLAF, JOE E. ET AL: "Purification and properties of deacetoxycephalosporin C synthase from recombinant Escherichia coli and its comparison wit the native enzyme purified from Streptomyces clavuligerus"  J. BIOL. CHEM. (1989), 264(17), 10219-27 CODEN: JBCHA3; ISSN: 0021-9258, 1989, XP002095823	1
Υ	see the whole document	2,3, 21-26
Х	BALDWIN J E ET AL: "HIGH-LEVEL SOLUBLE EXPRESSION AND PURIFICATION OF DEACETOXYCEPHALOSPORIN C-DEACETYLCEPHALOSPORIN C SYNTHASE." BIOORG MED CHEM LETT, (1992) 2 (7), 663-668. CODEN: BMCLE8. ISSN: 0960-894X.,	1
Y	XP002095824 see the whole document	2,3, 21-26
X Y	EP 0 366 354 A (LILLY CO ELI) 2 May 1990 see the whole document	1 2,3, 21-26
x⁄	BALDWIN J E ET AL: "HIGH-LEVEL SOLUBLE EXPRESSION AND PURIFICATION OF DEACETOXYCEPHALOSPORIN C-DEACETYLCEPHALOSPORIN C SYNTHASE." BIOORG MED CHEM LETT, (1992) 2 (7), 663-668. CODEN: BMCLE8. ISSN: 0960-894X., XP002095825	
Y	see the whole document	2,3, 21-26
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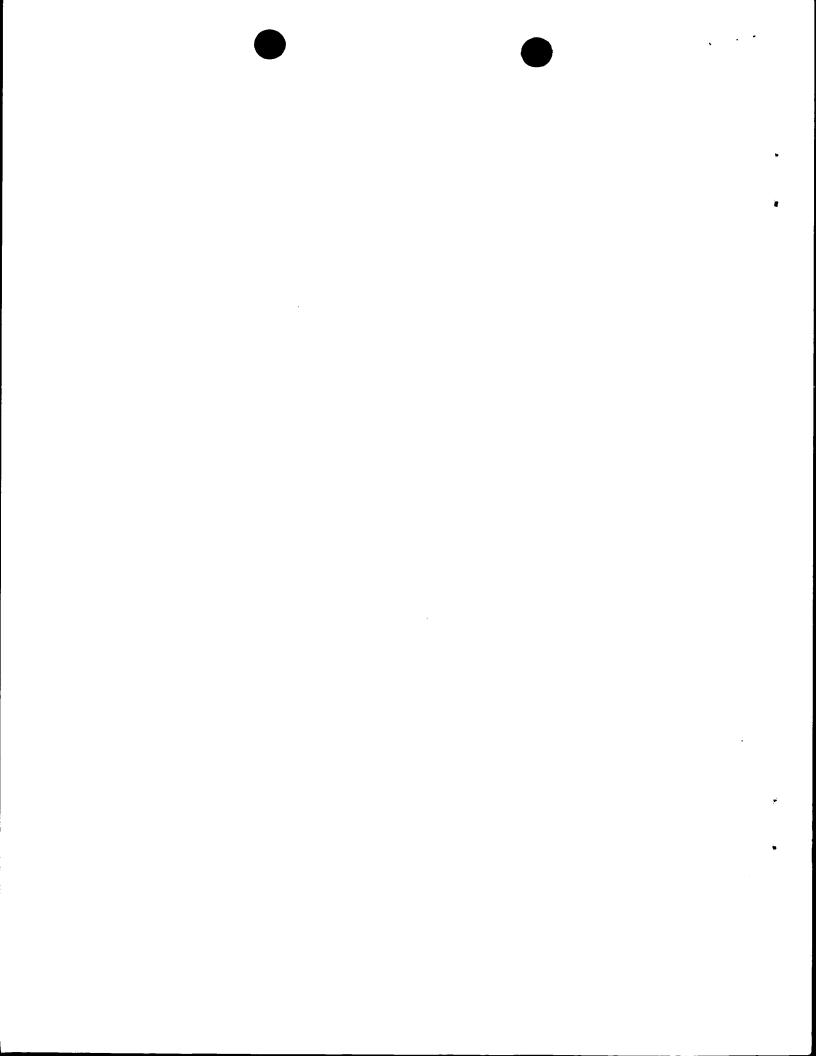
ategory '	ation) DOCUMENTS CONSIDERED TO BE RELEVANT  Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
	Ordinario accompany management of appropriately and accompany and accompany	
Ж	VALEGARD, KARIN ET AL: "Structure of a cephalosporin synthase" NATURE (LONDON) (1998), 394(6695), 805-809 CODEN: NATUAS;ISSN: 0028-0836,1998, XP002095826 see the whole document	1-11, 21-26
<b>y</b> ⁄	WO 98 16648 A (BALDWIN JACK EDWARD; CLIFTON IAN (GB); ISIS INNOVATION (GB); ROACH) 23 April 1998 see the whole document	1-26
	ROACH P L ET AL: "CRYSTAL STRUCTURE OF ISOPENICILLIN N SYNTHASE IS THE FIRST FROM A NEW STRUCTURAL FAMILY OF ENZYMES" NATURE, vol. 375, no. 6533, 22 June 1995, pages 700-704, XP002059796 cited in the application see the whole document	2,3, 21-26
/	SCOTT R A ET AL: "X-RAY ABSORPTION SPECTROSCOPIC STUDIES OF THE HIGH-SPIN IRON(II) ACTIVE SITE OF ISOPENICILLIN N SYNTHASE: EVIDENCE FOR FE-S INTERACTION IN THE ENZYME-SUBSTRATE COMPLEX" BIOCHEMISTRY, vol. 31, no. 19, 1992, pages 4596-4601, XP002067783 see the whole document	2,3,21-26
J	ROACH P L ET AL: "STRUCTURE OF ISOPENICILLINN SYNTHASE COMPLEXED WITH SUBSTRATE AND THE MECHANISM OF PENICILLIN FORMATION" NATURE, vol. 387, no. 6635, 19 June 1997, pages 827-830, XP002067787 cited in the application see the whole document	2,3, 21-26
V	WO 97 20053 A (GIST BROCADES BV ;UNIV OXFORD (GB); SUTHERLAND JOHN DAVID (GB); BO) 5 June 1997 cited in the application see the whole document	
ij	EP 0 532 341 A (MERCK & CO INC) 17 March 1993 cited in the application see the whole document	

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C.(Continu	ation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category '	Citation of document, with indication where appropriate, of the relevant passages		Relevant to claim No.
A	N. SHIBATA ET AL.:  "Adipoyl-6-aminopenicillanic acid is a substrate for deacetoxycephalosporin C synthase (DAOCS)."  BIOORGANIC & MEDICINAL CHEMISTRY LETTERS, vol. 6, no. 113, 1996, pages 1579-1584, XP002095827 cited in the application see the whole document		

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# INTERNATIONAL SEARCH REPORT

onal Application No PCT/GB 98/03860

Patent document cited in search repor	t	Publication date	Patent family member(s)	Publication date
EP 0366354	Α	02-05-1990	US 5082772 A DE 68925338 D DE 68925338 T DK 521489 A ES 2082787 T GR 3018596 T IL 92079 A JP 2242675 A	21-01-1992 15-02-1996 05-06-1996 25-04-1990 01-04-1996 30-04-1996 26-08-1994 27-09-1990
WO 9816648	Α	23-04-1998	NONE	
WO 9720053	Α	05-06-1997	AU 1097297 A EP 0863989 A GB 2323361 A	19-06-1997 16-09-1998 23-09-1998
EP 0532341	A	17-03-1993	US 5318896 A AT 173017 T AU 657787 B AU 2354292 A BG 98643 A CA 2077921 A,C CN 1075336 A CZ 9400532 A DE 69227494 D EP 0843013 A FI 941135 A HU 69801 A IL 103076 A JP 7501931 T KR 132440 B MX 9205175 A NO 940848 A NZ 244236 A PL 174984 B	07-06-1994 15-11-1998 23-03-1995 18-03-1995 12-03-1993 18-08-1993 17-08-1994 10-12-1998 20-05-1998 10-03-1994 28-09-1995 31-10-1996 02-03-1995 14-04-1998 28-02-1994 10-03-1994 25-03-1994 30-10-1998

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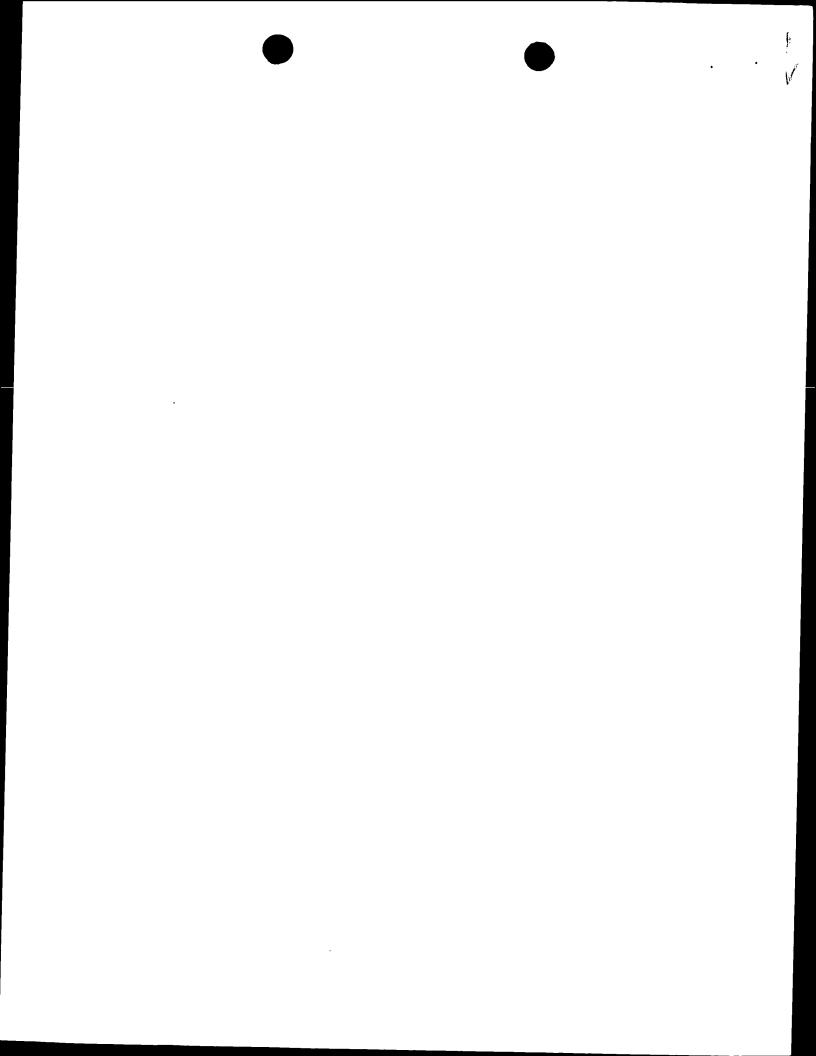
# **PCT**

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REC'D	30	MARS	2000
WIPO			PCT

# INTERNATIONAL PRELIMINARY EXAMINATION REPORT

(PCT Article 36 and Rule 70)

applicant's or		le reference	FOR FURTHER ACTIO	See Notific	cation of Transmittal of International y Examination Report (Form PCT/IPEA/416)
PP/2560 PC			International filing date (day/n	nonth/vear)	Priority date (day/month/year)
nternational a		n No.	1	,011a ii y = 0.17	24/12/1997
CT/GB98			24/12/1998		
nternational F C12N15/52		assification (IPC) or na	tional classification and IPC		
Applicant	_				
		N LIMITED et al.			
and is t	ransmit	ted to the applicant	according to Afficie 30.		ternational Preliminary Examining Authority
			f 6 sheets, including this co		
_			ed by ANNEXES, i.e. sheets asis for this report and/or sh 507 of the Administrative Ins	5 <del>6</del> (3 00)1101111119	ion, claims and/or drawings which have rectifications made before this Authority the PCT).
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These	annexe	s consist of a total c	of 5 sheets.		
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3. This re	eport co ⊠ B	ntains indications re asis of the report	lating to the following items		en and industrial applicability
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3. This re	eport co	ntains indications re asis of the report riority on-establishment of ack of unity of invent leasoned statement itations and explana	lating to the following items opinion with regard to nove tion under Article 35(2) with reg tions suporting such staten	lty, inventive st ard to novelty, i	
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3. This real limits in the second sec	eport co	ntains indications re asis of the report riority on-establishment of ack of unity of inven leasoned statement itations and explana certain documents of certain defects in the	lating to the following items opinion with regard to nove tion under Article 35(2) with reg tions suporting such staten cited e international application on the international applica	elty, inventive st ard to novelty, i ent tion	nventive step or industrial applicability;
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3. This read of the second of	eport co	ntains indications reasis of the report riority fon-establishment of ack of unity of inventeasoned statement itations and explanations and explanations and explanations defects in the certain defects in the certain observations of the demand	lating to the following items opinion with regard to nove tion under Article 35(2) with reg ations suporting such staten sited international application on the international applica	elty, inventive st ard to novelty, i ent tion	on of this report  2.7. 03.00
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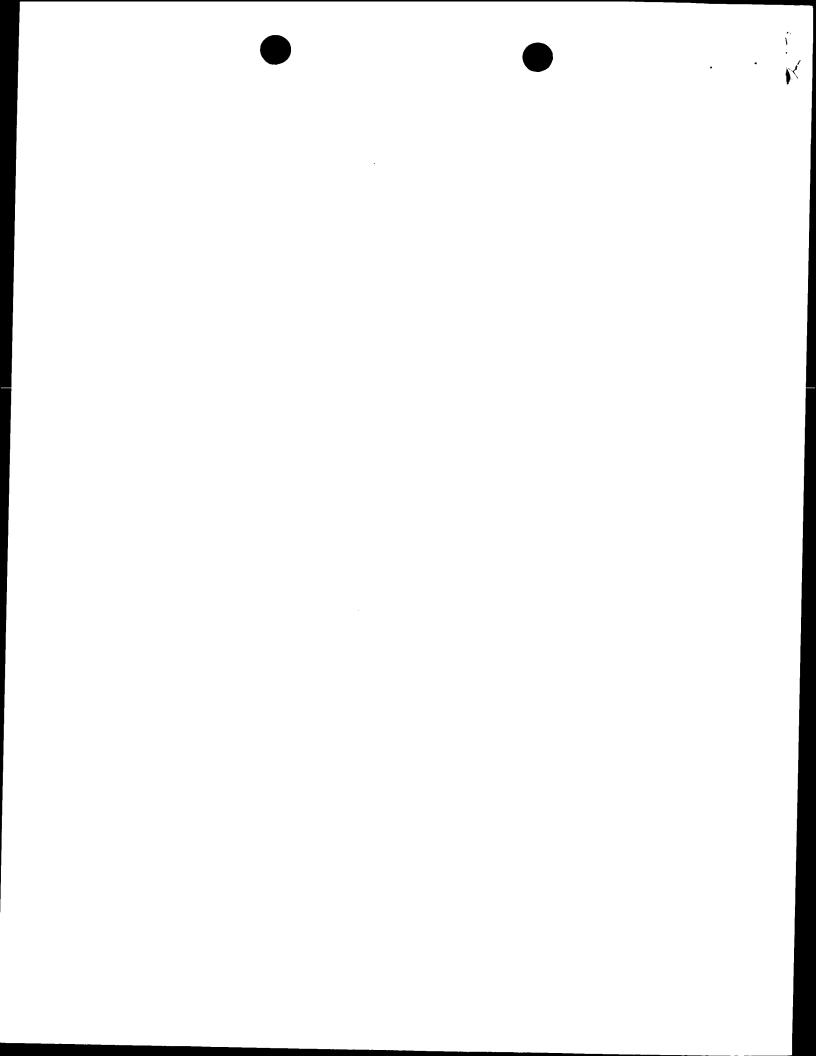
# INTERNATIONAL PRELIMINARY EXAMINATION REPORT

International application No. PCT/GB98/03860

# I. Basis of the report

 This report has been drawn on the basis of (substitute sheets which have been furnished to the receiving Office in response to an invitation under Article 14 are referred to in this report as "originally filed" and are not annexed to the report since they do not contain amendments.):
 Description, pages:

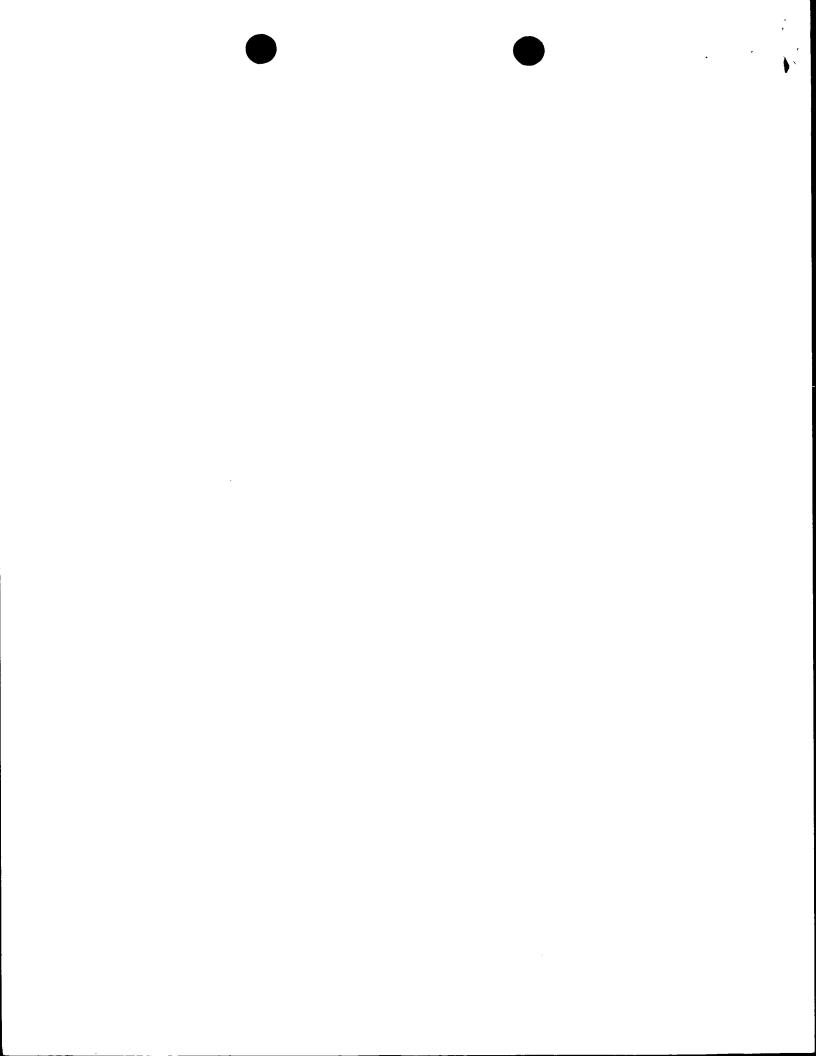
	Desc	ription, pages:					
	1-164		as originally filed				
	<b>Clain</b> 1-26	ns, No.:	as received on	03/01/2000	with letter of	29/12/1999	
	<b>Draw</b>	vings, sheets: 7/2	as originally filed				
2.	The	amendments hav	ve resulted in the cancella	ation of:			
		considered to go	pages: Nos.: sheets: Deen established as if (so Deyond the disclosure a	ome of) the amendme is filed (Rule 70.2(c)):	nts had not been	n made, since they have beer	า
			of opinion with regard				
7	he quer to b	uestions whether e industrially app	the claimed invention ap licable have not been ex	pears to be novel, to amined in respect of:	involve an invent	tive step (to be non-obvious)	•
		the entire intern	national application.				
	×	claims Nos. 4-2	26.				
Ī	becau	ıse:					



# INTERNATIONAL PRELIMINARY EXAMINATION REPORT

International application No. PCT/GB98/03860

		the said international application, or the said claims Nos. relate to the following subject matter which does not require an international preliminary examination ( <i>specify</i> ):
		the description, claims or drawings (indicate particular elements below) or said claims Nos. are so unclear that no meaningful opinion could be formed (specify):
	×	the claims, or said claims Nos. 4-26 are so inadequately supported by the description that no meaningful opinion could be formed.
		no international search report has been established for the said claims Nos
IV.	Lac	k of unity of invention
1.	In re	esponse to the invitation to restrict or pay additional fees the applicant has:
		restricted the claims.
		paid additional fees.
		paid additional fees under protest.
		neither restricted nor paid additional fees.
2.	⊠	This Authority found that the requirement of unity of invention is not complied and chose, according to Rule 68.1, not to invite the applicant to restrict or pay additional fees.
3.	This	Authority considers that the requirement of unity of invention in accordance with Rules 13.1, 13.2 and 13.3 is
		complied with.
	×	not complied with for the following reasons:
		see separate sheet
4.		sequently, the following parts of the international application were the subject of international preliminary mination in establishing this report:
	☒	all parts.
		the parts relating to claims Nos





International application No. PCT/GB98/03860

- V. Reasoned statement under Article 35(2) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement
- 1. Statement

Novelty (N)

Yes:

Claims 1-3

No:

Claims

Inventive step (IS)

Yes: No:

Claims

Industrial applicability (IA) Yes:

Claims 1-3

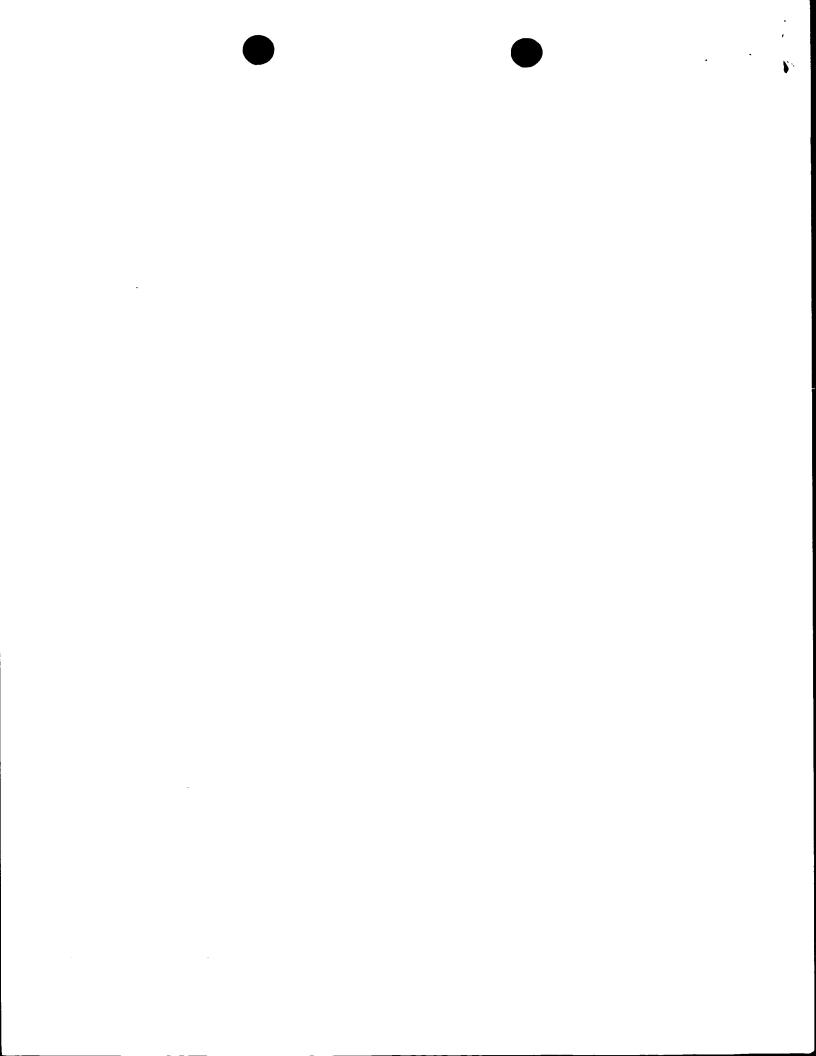
Claims 1-3

No:

Claims

2. Citations and explanations

see separate sheet



### INTERNATIONAL PRELIMINARY **EXAMINATION REPORT - SEPARATE SHEET**

- The present application relates to a cephalosporin synthase in crystalline form, the 1. use thereof, various modified cephalosporin synthases, genes encoding these enzymes, host cells, use of the host cells for producing and various methods related to · the use of the three dimensional structure of the DAOCS.
- The following objections apply to present set of claims. 2.

#### 2.1 item IV:

The present set of claims lacks unity as required by Rules 13.1-13.3 PCT, since it comprises several groups of claims (and even alternatives within one claim) which are not connected by the same inventive concept (see especially the various mutants claimed in claims 12 and 13 but also the different three dimensional structures). In view of the other defects contained in the set of claims, this authority, at present, will not prosecute this objection.

#### 2.2 item III:

The applicant has determined the three dimensional structure of DAOCS alone and in a complexed form with Fe(II) and 2-oxoglutarate.

On the basis of said structure the applicant drafted some speculative claims which relate to the use of said structure (or the information retrieved from said structure) and to modified enzymes. However, none of said claims is supported by experimental data. Therefore, in the absence of any experimental data the claimed subject-matter must be regarded as being totally speculative.

#### 2.3 Item V:

Insofar as claims which are supported by experiments are concerned i.e. claims 1 to 3 (partially) an inventive step has to be denied. In fact the determination of the three dimensional structure of an enzyme in the absence or presence of its substrate in order to identify an active center etc is routine for a person skilled in the art. This has inter alia been verified with a closely related enzyme namely IPNS (see D1: Nature, vol. 375, No. 6533, 1995, pages 700-704). However, should this be incorrect, said claims are not enabled because the application does not contain any description of the preparation of this structure. Thus either claims 1-3 lack an inventive step according to Article 33(3) PCT or they are inadmissible under Article 5 PCT.

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# INTERNATIONAL PRELIMINARY

International application No.

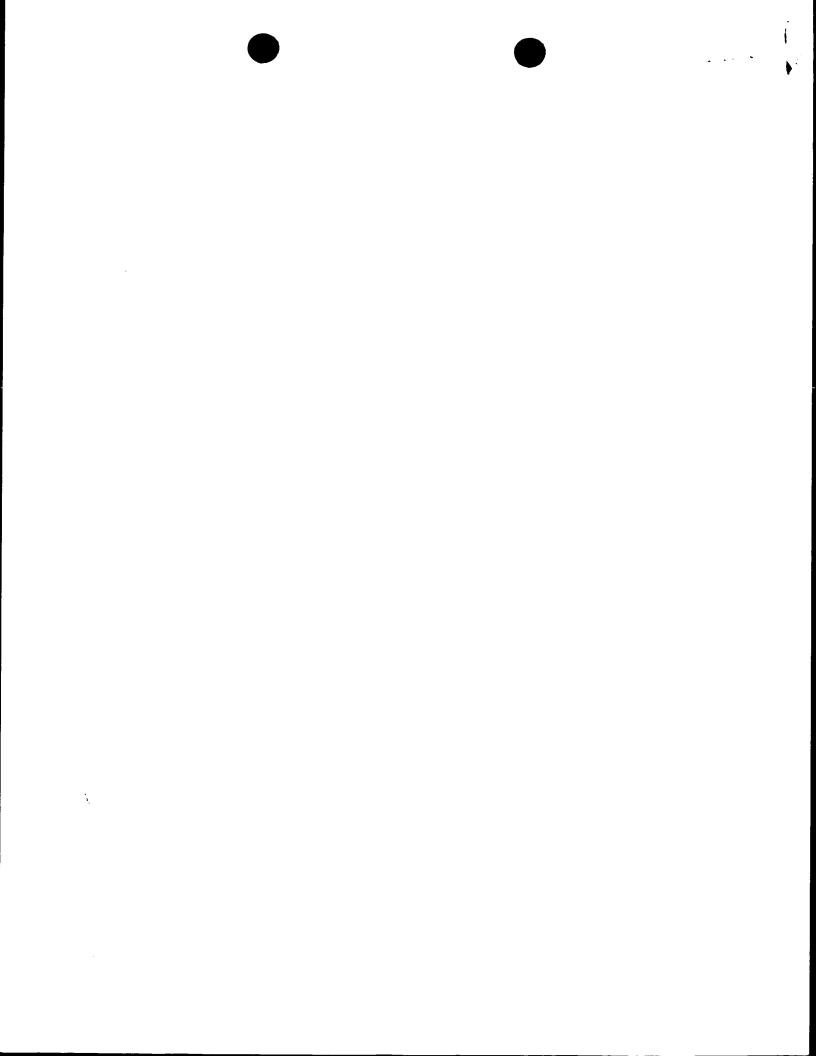
PCT/GB98/03860

**EXAMINATION REPORT - SEPARATE SHEET** 

Anything which might constitute a contribution to the art, namely the use of the three dimensional structure to produce modified enzymes which serve a special technical purpose confirmed by experimental data, has not been shown in the application.

#### 2.4 Summary:

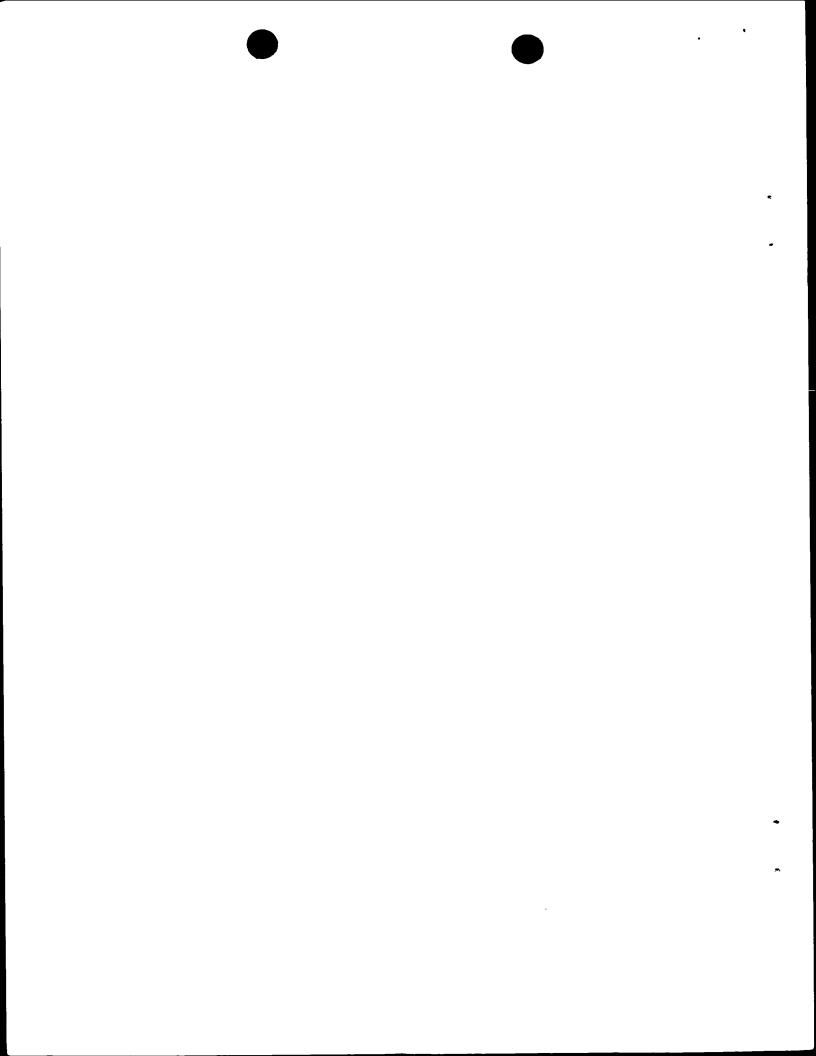
Therefore present claims either lack an inventive step (Article 33(2) PCT) i.e present claims 1-3 or lack support as required by Article 6 PCT i.e. present claims 4-26.



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IPEA/\_\_EP

**PCT** 

CHAPTER II

#### **DEMAND**

under Article 31 of the Patent Cooperation Treaty:

The undersigned requests that the international application specified below be the subject of international preliminary examination according to the Patent Cooperation Treaty and hereby elects all eligible States (except where otherwise indicated).

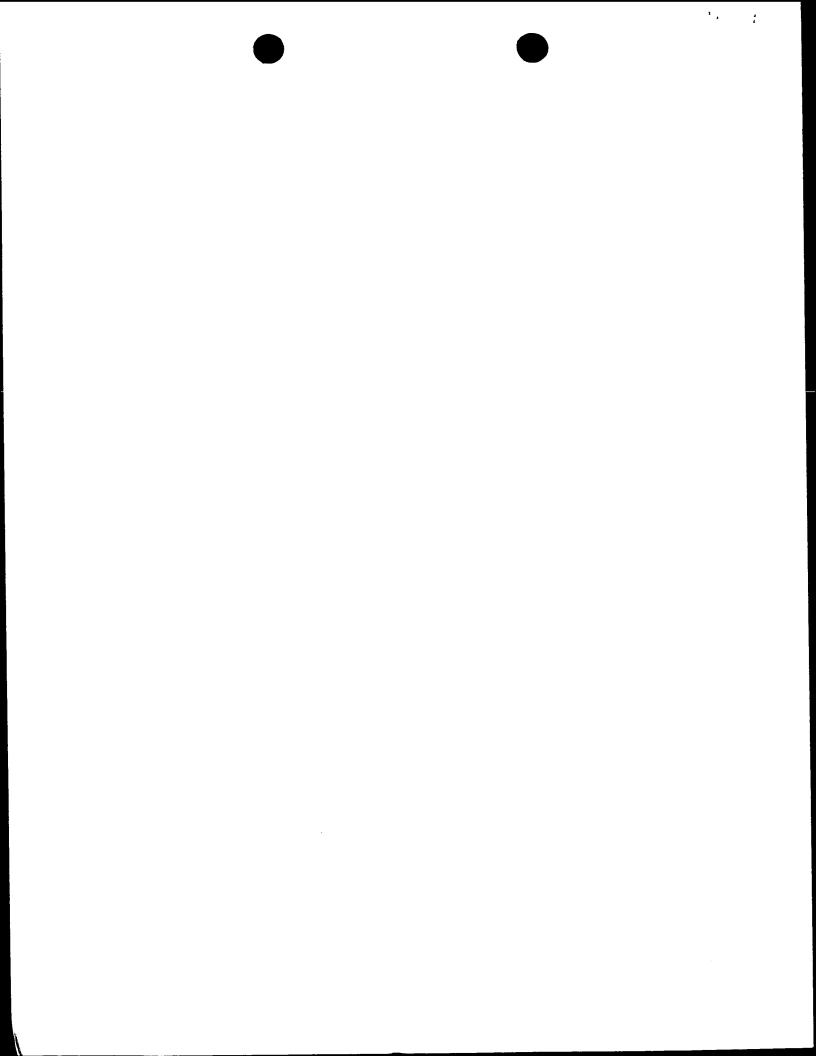
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Identification of IPEA		Date of receipt of D	DEMAND
Box No. I IDENTIFICATION OF T	HE INTERNATIONAL	APPLICATION	Applicant's or agent's file reference PP/2560 PCT
International application No. PCT/GB98/03860	International filing da	•	(Earliest) Priority date (day/montic year) 24 December 1997 (24-12-97)
Title of invention  MODIFIED DEACETOXYCEPHALOSPORIA	N C SYNTHASE (DAOCS	) AND X-RAY STRUC	CTURE
Box No. II APPLICANT(S)		· · · · · · · · · · · · · · · · · · ·	· · · · · · · · · · · · · · · · · · ·
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International application No. PCI/GB98/03860

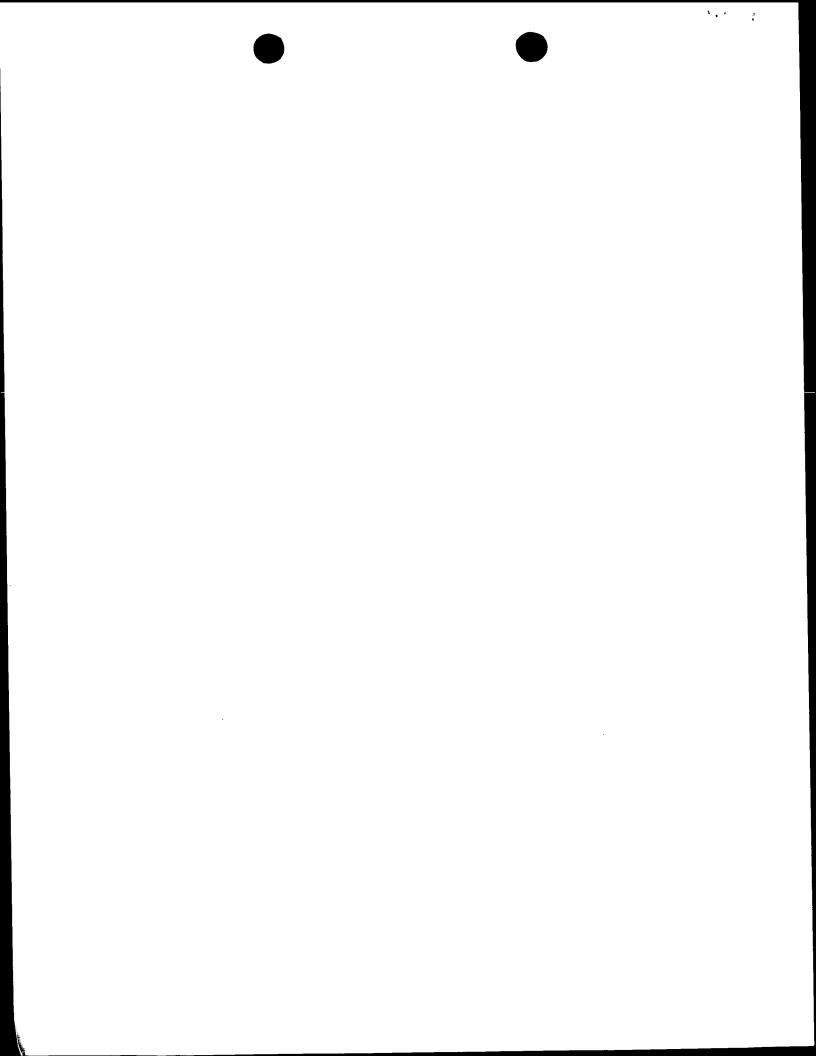
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### Sheet No. . 3.

International application No. PCT/GB98/03860

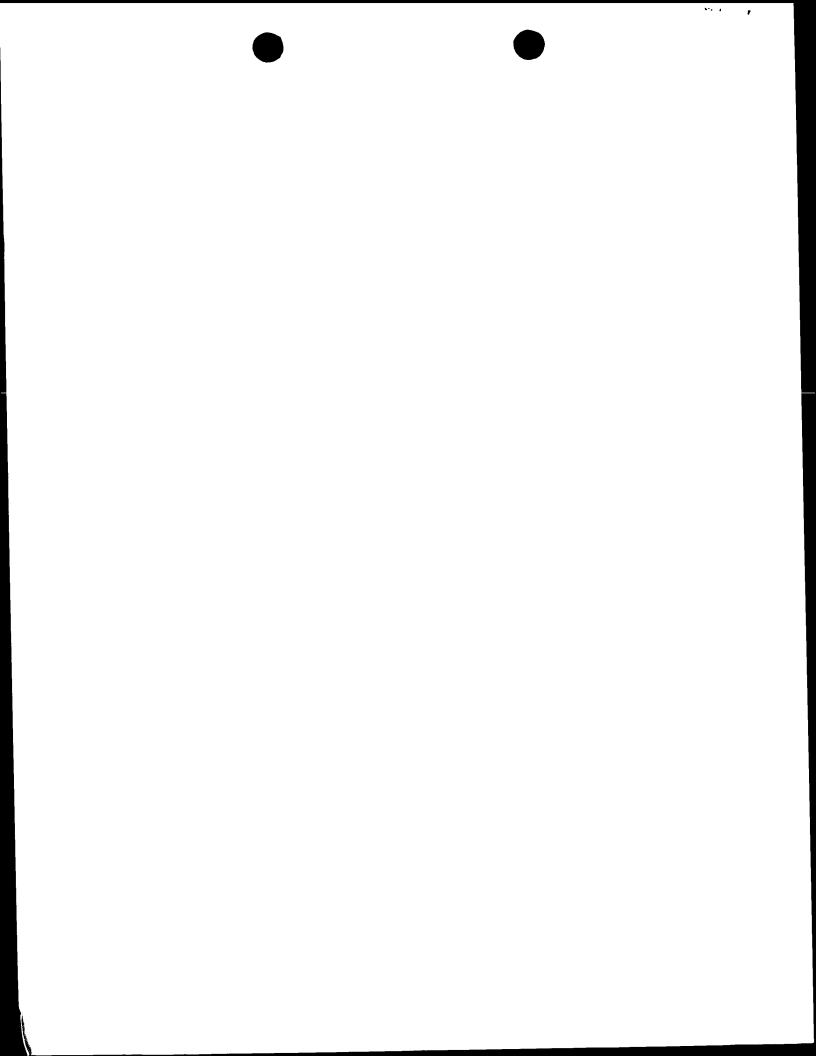
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International application No.

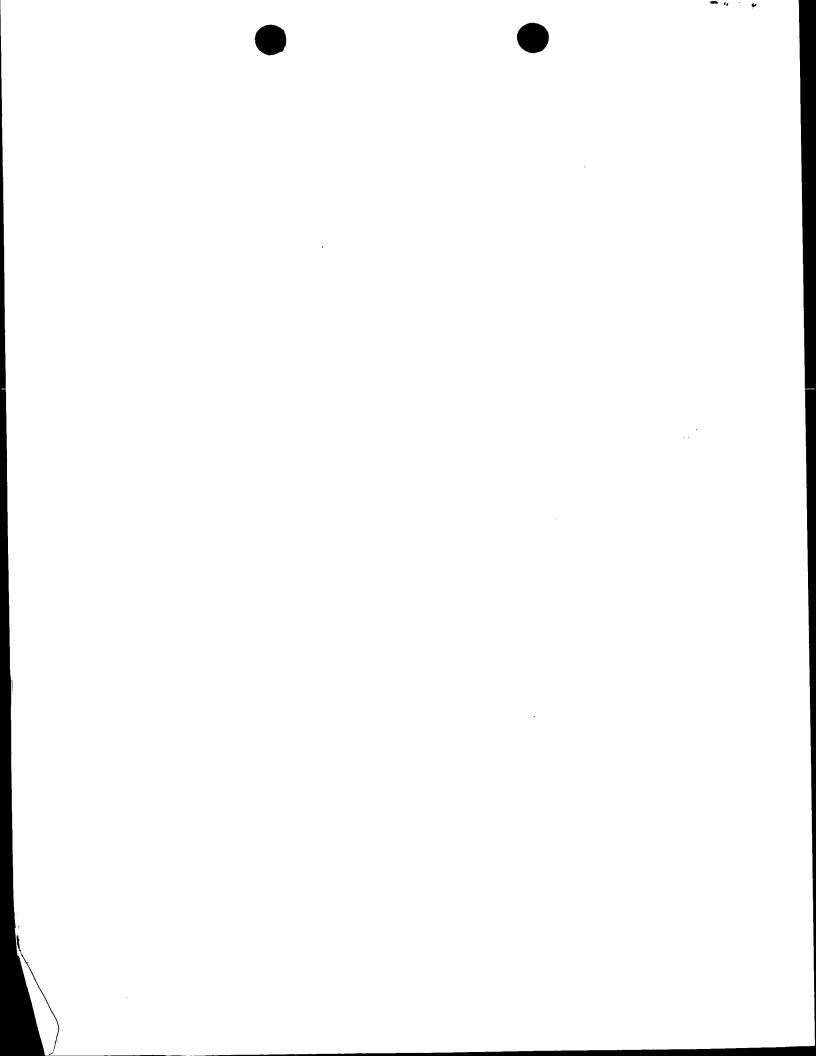
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and an arrangement appropriate as originally fried	
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the claims as originally filed	
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the drawings as originally filed	
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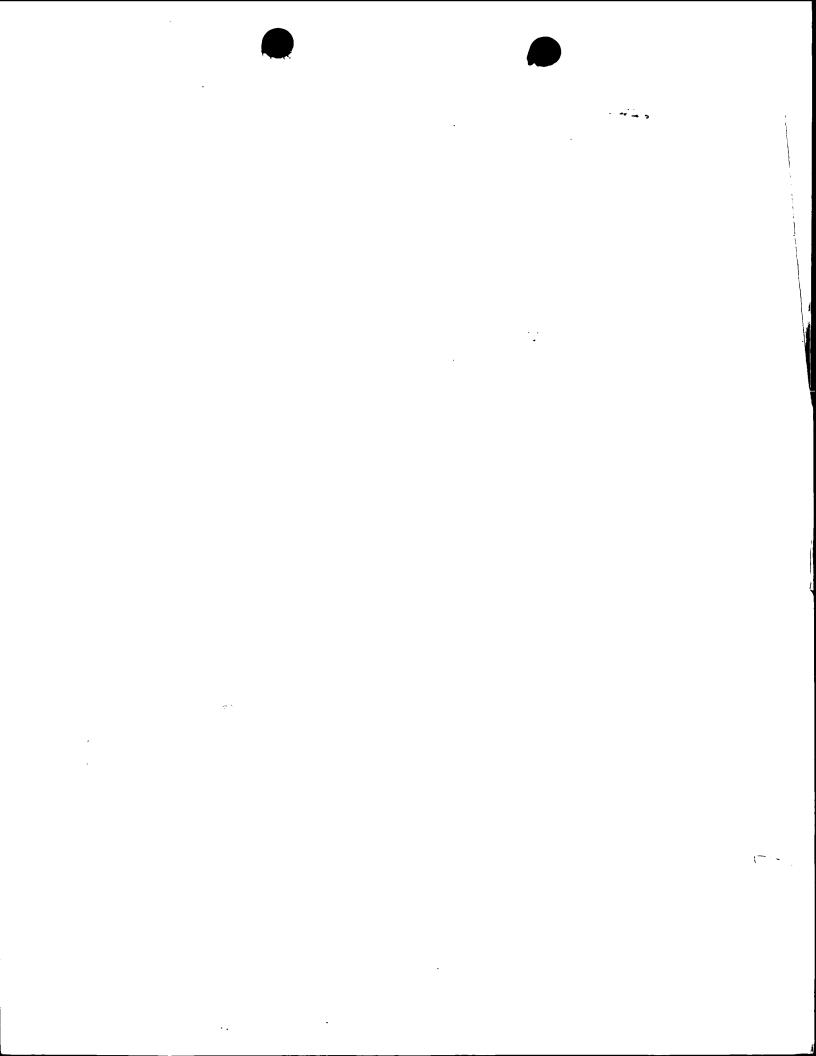
With international search report.

(54) Title: MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

(57) Abstract

Three-dimensional crystal structure(s) of deacetoxycephalosporin C synthase (DAOCS) are described. The X-ray co-ordinates provide precise 3-dimensional information of amino acids within the structure of DAOCS. Some of these are in complexes with iron and/or substrates. Information from the structures is used to modify enzymes of the cephalosporin biosynthesis pathway including DAOCS, deacetylcephalosporin C synthase DAOC/DACS, such that they accept unnatural substrates (e.g. penicillins G, V) in order to improve the production of beta-lactam antibiotics. The structures may be used to predict the structures of other 2-oxoglutarate dependent enzymes, thereby allowing the design of inhibitors, and new catalysts for the production of e.g. oxidised amino acids/peptides. Specific modifications of amino acid residues are proposed and exemplified.

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532 Rec'd PCT/PTO 23 JUN 2000

# MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

Penicillin and cephalosporin antibiotics are produced either directly by fermentation or by modification of fermentation derived materials containing a beta-lactam ring. The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and reviewed (J. E. Baldwin and C. J. Schofield, in 'The Chemistry of β-lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Ingolia and Queener, Med. Res. Rev., 1989, 9, 245-264; Aharonowitz, Cohen and Martin, Ann. Rev. Microbiol., 1992, 46, 461-495; Schofield, Bycroft, Baldwin, Hadju, Roach, Current Opinion in Structural Biology, 1997, 7, 857-864) and includes the

- following steps (Figure 1):

  1. Conversion of the tripeptide: <u>L</u>-δ-α-aminoadipoyl-<u>L</u>-cysteinyl-<u>D</u>-valine (ACV) to isopenicillin N in a step catalysed by isopenicillin N synthase (IPNS). This step is common to both penicillin and cephalosporin
  - biosynthesis.
- In some organisms (e.g. Penicillium chrysogenum and Aspergillus nidulans) isopenicillin N is converted by exchange of its ½-δ-α-aminoadipoyl side chain to penicillins with other side chains, which are normally more hydrophobic than the side chain of isopenicillin N. This conversion is catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins may be commercially produced via fermentation under the appropriate conditions.
  - 3. In other organisms (e.g. *Streptomyces clavuligerus* and *Cephalosporium acremonium*) isopenicillin N is epimerised to penicillin N.
- This reaction is catalysed by an epimerase enzyme.

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- 4. In some organisms (e.g. S. clavuligerus and C. acremonium) penicillin N is converted to DAOC. This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. Streptomyces clavuligerus) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. C. acremonium).
- 5. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. *S. clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in *C. acremonium* DAC may be converted to cephalosporin C and in *Streptomyces spp*. DAC may be converted to cephamycin C. The genes encoding for each of the enzymes catalysing steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins and their biosynthetic intermediates are useful as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or intermediates used in the preparation of cephalosporins, e.g. penicillins (including penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, *e.g.* Cefachlor.

The enzymes IPNS, DAOCS, DACS and DAOC/DACS are members of an extended family of Fe(II) utilising oxidase and oxygenase enzymes. Most of this family (including DAOCS, DACS and DAOC/DACS) utilise a 2-oxo acid (normally 2-oxoglutarate) as a cosubstrate in addition to dioxygen and the 'prime' substrate (e.g. penicillin N in the case of DAOCS). Since IPNS, does not use 2-oxoglutarate, it has a substantially different mechanism to the 2-oxoglutarate dependent oxygenases, and this gives

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rise to a significantly different active site.

#### The Invention

This invention is based on the determination of the three dimensional crystal structure of DAOCS and the information and developments which come from it. The X-ray co-ordinates provide very detailed 3-dimensional information on the relationships between amino acid residues in the structure of DAOCS and on the binding modes of the Fe-cofactor and the substrates to DAOCS. The structure allows the modification of DAOCS and related enzymes of penicillin and cephalosporin biosynthesis (including DACS and DAOC/DACS) in order to alter their substrate and product selectivities. Since the DAOCS structures are the first from the family of 2-oxoglutarate dependent dioxygenases they also allow for the design of new inhibitors of this family of enzymes. Previously partial overviews of the structures of IPNS complexed to manganese and IPNS complexed to iron and ACV were reported (Roach et al., Nature, 1995, 375, 700-704; Roach et al., Nature, 1997, 387, 827). The structures, as defined by their X-ray co-ordinates, of IPNS complexed to manganese and in complexes with iron, ACV and/or substrate analogues have been reported in Baldwin, Hajdu, Roach, Hensgens, Clifton, GB 9621486.1- (Oxygenase Enzymes and Method).

Procedures have been developed for the production of 7-aminodeacetoxycephaosporin C (7-ADCA) in which recombinant *P. chrysogenum* strains into which the DAOCS gene has been introduced are used for the production of cephalosporins. In particular if adipic acid is added to these recombinant strains adipoyl-6-APA is produced, which is converted by DAOCS into adipoyl-7-ADCA from which the adipoyl side chain can be removed (EPA-A-0532341, Shibata *et al.*, Bioorg. Med. Chem. Letts, 1996, 6, 1579-1584).

The IPNS gene sequence (and therefore the amino acid

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sequence) is related but significantly different to those of DAOCS, DACS, DAOC/DACS. It is likely that gross elements of the fold (i.e. significant elements within the 3-dimensional structure) of these enzymes will be conserved but that the active site architecture will be very significantly different. Structural elements conserved are likely to include the beta-barrel 'jelly roll' core and certain alpha-helices (including alpha helix-10, as defined in Roach *et al.*, Nature, 1995, 375, 700-704). The degree of similarity is insufficient to define the precise structure of DAOCS, DACS, or DAOC/DACS from the IPNS structures. To date no models of DAOCS,

DACS, or DAOC/DACS based on the IPNS structure have been reported. Nor have any detailed studies on substrate binding of these enzymes been reported. One report (WO 97/20053) claims the use of products resulting from modification of certain residues in DAOCS for the improved conversion of penicillin G to phenyl acetyl (G)-7-aminocephalosporanic acid.

The three-dimensional structure of DAOCS is defined by the X-ray co-ordinates set out below (Structure A).

Also set out below is a high resolution crystal structure of a complex of prokaryotic DAOCS from *S. clavuligerus* with Fe(II) and 2-oxoglutarate (Structure B).

In part the present invention relates to the use of the structures of DAOCS in order to make modifications to it or DACS or DAOC/DACS in order that the modified enzymes catalyse the conversion of unnatural penicillins (e.g. penicillin G and penicillin V) to cephalosporins more efficiently than the wild-type enzyme. Further aspects of the invention relate to the use of the DAOCS structure in order to produce unnatural products in micro-organisms. Such products include exomethylene cephalosporins, with or without alpha-aminoadipoyl or hydrophobic side chain (e.g. phenylacetyl or phenoxyacetyl). Thus one aspect of this invention refers to the use of the structure of DAOCS for modifying DAOCS

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(or the closely related enzymes DACS or DAOC/DACS) in order to:

- (i) permit the enzyme to accept (or accept more efficiently) unnatural penicillin substrates for the preparation of new or commercially valuable antibacterial materials.
- (ii) enable the modified enzyme to produce unnatural (e.g. exomethylene cephams) or optimise the production of minor products (e.g. 3-β-hydroxycephams) for use as antibacterials or as intermediates in the preparation of antibacterials or commercially valuable compounds.

In another aspect this invention provides modified enzymes that result from application of the aforementioned techniques. These are enzymes having significant (as defined below) sequence and thus structural similarity with DAOCS. Thus, structures of these enzymes may be predicted on the basis of the DAOCS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a major part of DAOCS. Previous sequence comparisons (Roach et al., Nature, 1995, 375, 700), using pairwise comparisons of the sequences followed by single linkage cluster analysis show that IPNS, DAOCS, DACS and DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Scores over 5.0 and preferably over 6.0 indicate that the sequence alignments will be correct within all or most of the protein secondary structural elements (Barton, Methods in Enzymol., 1990, 183, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity or % similarity of amino acids possessing side chains with similar physicochemical properties (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Thus, on the basis of sequence comparisons it is possible to predict the structure of one enzyme (e.g. DACS or DAOC/DACS) from another closely related enzyme (e.g. DAOCS). Further, it is recognised that although two enzymes may have structures in which secondary structural elements are

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largely or wholly conserved, differences in the structures of the two enzymes may result from the side chains of the amino acids forming the secondary structural elements. The effect of these differences, which alter the substrate/product selectivities of the compared enzymes, is predictable once the three-dimensional structure of one of the enzymes is known.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Modifications of this kind will permit the expansion of penicillin V or penicillin G to the corresponding cephalosporins. To achieve this it is desirable to increase the kcat/Km for the mutant as compared to the wild type DAOCS. Kinetic results indicate that apparent kcat values for penicillin N and penicillin G are similar but that Km is much higher for penicillin G. Thus based on these analysis, a decrease in the binding constant of DAOCS for penicillin G should make it possible to increase kcat/Km for penicillin G.

The side chain binding pocket of DAOCS is made of residues from different parts of the peptide chain, so it is likely that more than one residue will have to be altered to make a better penicillin G/V expander. Nevertheless some residues are more important than others. Examination of the interactions between the last few C-terminal residues (Thr-308 to Ala-311) of one DAOCS molecule and the active site of another in the crystal structure, suggests a binding mode for the penicillin nucleus which

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is shown in Figure 2 of the accompanying drawings. The penam C-3 carboxylate group probably occupies an analogous position to that of Ala-311 from a symmetry related molecule in the active site, forming electrostatic interactions with Arg-162 and Arg-160. The side chain of Arg-160 may also form a hydrogen bonding interaction with the  $\beta$ -lactam carbonyl.

It needs to be borne in mind that protein specificity is generally controlled by more than one amino acid. To alter the specificity of a protein in a major way is likely to require more than one of the mutational changes suggested below, although each of the mutations will contribute. With this in mind, preferred residues to modify for the expansion of a penicillin are as follows:

- a) Arg-266. This residue binds with the  $\alpha$ -aminoadipate side chain of the natural substrate and should be changed to a residue of more hydrophobic character, e.g. Phe, Ala, Val, Leu, Ile.
- b) Thr-72. This should be changed to a hydrophobic residue e.g. Val, Leu, Ile, Phe, Ala, to help bind the hydrophobic side chain of penicillin G. It should be effective in combination with other mutants.
- c) Arg-74 may be usefully changed to a neutral or hydrophobic residue (Phe, Tyr, Val, Leu, Ile, Ala). Modification of Arg-75 may be necessary in addition because it forms a hydrogen-bonding network with Arg-74.
- d) Glu-156. This residue binds with the  $\alpha$ -aminoadipate side chain. It should be changed to one of Ala, Val, Leu, Ile, Phe, Tyr, Trp, Asn, Gln, Ser.
- e) The side chains of Leu-158, Asn-301 and Tyr-302 form part of the binding pocket for the penicillin side chain and can be usefully modified to more hydrophobic character.
  - f) Asn-304. This residue binds the amide linking the side chain to the penam nucleus. Modification is effected to expand penicillins with shortened or no side chains (e.g. to Asp or Glu for 6-Apa).

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Note that other changes may be used to construct part or all of a side chain binding pocket via hydrogen bonding or other interactions.

The insertion or deletion of residues into the DAOCS sequence may also be of use in constructing a hydrophobic binding pocket for the penicillin side chain. Insertion of hydrophobic residues into the C-terminal region (residue 300-311 and in particular 301-303) may assist in the construction of a hydrophobic binding pocket for penicillin side chains.

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In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Asn304, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Further discussion of this aspect may be found in Nature Volume 394, pages 805-809 published on 20 August 1998 and incorporated by reference herein.

20 Another aspect of the invention refers to the use of the structure of DAOCS in order to modify its active site (or that of a structurally related 2-oxoglutarate dependent dioxygenase) in order that the modified enzyme accepts non beta lactam substrates in order to produce oxidised compounds of value. Oxidised amino acids (e.g. 4-hydroxyprolines, hydroxylysines, hydroxyaspartic acids and others) are useful as synthetic intermediates in the production of valuable materials. Using the structure of DAOCS specific residues can be targeted for modification in order that the modified enzyme can be used to produce oxidised amino acids or peptides. The process may include modification of the following residues:

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Arg74, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304, Ile88, Arg162, Phe164, Met180, Thr190, Ile192, Pro241, Val245, Val262, Ile305, Arg306, Arg307.

Another aspect of the invention refers to the use of the DAOCS structure for the design of selective inhibitors of 2-oxoglutarate dependent dioxygenases. The 2-oxoglutarate dependent dioxygenase prolyl 4-hydroxylase has been the target of inhibition in order to provide a therapeutic treatment for fibrotic diseases (e.g. liver cirrhosis, arthritis). However, no inhibitors are in clinical use, probably because it is difficult to achieve selective inhibition of the target enzyme for inhibition over other enzymes (including 2-oxoglutarate dependent enzymes). The structure of DAOCS provides a template for the design of inhibitors of 2-oxoglutarate dependent dioxygenases.

Set out below are two high resolution crystal structures for DAOCS from *S. clavuligerus*: the structure of the iron-free apoenzyme (Structure A) and the structure of the complex with Fe(II) and 2-oxoglutarate (Structure B). The results imply a mechanism by which the enzyme-Fe(II) complex reacts with 2-oxoglutarate and dioxygen to give the reactive ferryl species, a process common to many non-haem oxygenases. Other notable 2-oxoacid-dependent ferrous enzymes are prolyl hydroxylase, involved in collagen biosynthesis, gibberellin 3β-hydroxylase, a mutation of which influences stem length in plants, and clavaminic acid synthase, involved in the biosynthesis of the β-lactamase inhibitor, clavulanic acid. Within the family of 2-oxoacid-dependent enzymes, DAOCS belongs to a sub-family, the members of which show sequence similarity with IPNS and 1-aminocyclopropane-1-carboxylate oxidase (the ethylene forming enzyme), enzymes that do not use a 2-oxoacid in catalysis.

The iron-free form of DAOCS crystallises in space group R3

as a crystallographic trimer. The main chain of the protein folds into a conserved jelly roll core with flanking helices.

Co-ordinates and structure factors have been deposited with the Protein Data Bank (entries 1rxg, and r1rxgsf for the Fe(II)-2-oxoglutarate complex).

### LEGENDS TO FIGURES.

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Figure 1: the biosynthetic pathway to the penicillins and cephalosporins.

Figure 2 is a view of the active site of DAOCS showing 2-oxoglutarate binding to the iron and proposed penicillin N binding. Interactions with the side chains of certain amino acid residues are indicated by arrows.

Structure A is a three-dimensional structure of DAOCS.

Structure B is a high resolution crystal structure for prokaryotic DAOCS from *S. clavuligerus* as a complex with Fe(II) and 2-oxoglutarate.

The peptide sequence of DAOCS (with the numbering used herein) is set out below:

Met Asp Thr Thr Val Pro Thr Phe Ser Leu 10 Ala Glu Leu Gln Gln Gly Leu His Gln Asp 20 Glu Phe Arg Arg Cys Leu Arg Asp Lys Gly 30 Leu Phe Tyr Leu Thr Asp Cys Gly Leu Thr 40 Asp Thr Glu Leu Lys Ser Ala Lys Asp Leu 50 5 Val Ile Asp Phe Phe Glu His Gly Ser Glu 60 Ala Glu Lys Arg Ala Val Thr Ser Pro Val 70 Pro Thr Met Arg Arg Gly Phe Thr Gly Leu 80 Glu Ser Glu Ser Thr Ala Gln Ile Thr Asn 90 Thr Gly Ser Tyr Ser Asp Tyr Ser Met Cys 100 ΙÛ Tyr Ser Met Gly Thr Ala Asp Asn Leu Phe 110 Pro Ser Gly Asp Phe Gly Arg Ile Trp Thr 120 Gln Tyr Phe Asp Arg Gln Tyr Thr Ala Ser 130 Arg Ala Val Ala Arg Glu Val Leu Arg Ala 140 Thr Gly Thr Glu Pro Asp Gly Gly Val Glu 150 15 160 Ala Phe Leu Asp Cys Glu Pro Leu Leu Arg Phe Arg Tyr Phe Pro Gln Val Pro Glu His 170 Arg Ser Ala Glu Glu Gln Pro Leu Arg Met 180 Ala Pro His Tyr Asp Leu Ser Met Val Thr 190 Leu Ile Gln Gln Thr Pro Cys Ala Asn Gly 200 20 Phe Val Ser Leu Gln Ala Glu Val Gly Gly 210 Ala Phe Thr Asp Leu Pro Tyr Arg Pro Asp 220 230 Ala Val Leu Val Phe Cys Gly Ala Ile Ala 240 Thr Leu Val Thr Gly Gly Gln Val Lys Ala Pro Arg His His Val Ala Ala Pro Arg Arg 250 25 Asp Gln Ile Ala Gly Ser Ser Arg Thr Ser 260 270 Ser Val Phe Phe Leu Arg Pro Asn Ala Asp Phe Thr Phe Ser Val Pro Leu Ala Arg Glu 280 Cys Gly Phe Asp Val Ser Leu Asp Gly Glu 290 Thr Ala Thr Phe Gln Asp Trp Ile Gly Gly 300 30 Asn Tyr Val Asn Ile Arg Arg Thr Ser Lys 310 311 Ala

## STRUCTURE A

CRYST1	106.400	106 4	106.400					
SCALE1	0.009		•	71.100		90.00	90.00	120.00
SCALE2			0.0054	26	0.0000	00	0.0000	00
	0.000	0000	0.0108	52	0.0000	00	0.0000	00
SCALE3	0.000	0.000000			0.044005			
			0.00000		0.014065		0.00000	00

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MOTA	1	N	AMET	1	31.434	10.641	59.873	0 542	44 31
ANISOU	1	N	AMET	1	8315	2319	6203		*3454 - 791
$\mathtt{ATOM}$	2	CA	AMET	1	30.985	11.769	59.065	0.542	39 90
ANISOU	2	CA	AMET	1	9037	3006	3117	÷786	-1026 - 296
MOTA	3	С	AMET	1	30.472	12.900	59.956		28 97
ANISOU	3	С	AMET	1	4807	3113	3086	-421	-2189 -119
ATOM	4	0	AMET	1	29.961	12.670	61.055		28 12
ANISOU	4	0	AMET	1	3925	2381	4377	-402	-1097 7 4
MOTA	5	CB	AMET	1	29.970	11.328	58.023		34 85
ANISOU	5	CB	AMET	1	7877	3692	1672		1 - 3 7 3
MOTA	6	CG	AMET	1	28.626	12.015	57.903		
ANISOU		CG		1	7367	4873	2270	133	912 -1765
ATOM	7	SD		1	27.564	11.232	56.654	0.542	
ANISOU	7	SD		1	6146	7957	3827	-2344	1050 ~ 1326
ATOM	8	CE		1	28.129	11.973	55.135	0.542	27.10
ANISOU		CE	AMET	1	5030	2111	3155	2345	-1467 - 9
ATOM	9	N	AASP		30.592	14.105	59.425	0.268	30.20
ANISOU	-	N	AASP		4674	3022	3777	-1210	-782 - 383
MOTA	10	CA	AASP		29.993	15.322	59.963	0.268	34.22
ANISOU	10	CA	AASP		5567	2803	4633	-1106	-964 -525
ATOM	11	Ċ	AASP		28.494	15.268	59.655	0.268	33.34
ANISOU ATOM	11	C	AASP		5665	1997	5006	-314	-1457 877
ANISOU	12 12	0	AASP		28.099	15.650	58.551		
ATOM	13	O CB	AASP		6859	5248	4901	-1023	-1582 1631
ANISOU	13	CB	AASP AASP		30.629	16.528	59.281		
ATOM	14	CG			4424	3085	2361	322	-1794 582
ANISOU		CG	AASP	2	29.978	17.862	59.553		
ATOM	15		AASP		6456 28.995	2611	5389	-501	-608 -1114
ANISOU				2	6406	17.937 504 917	60.318		
ATOM	16		AASP	2	30.449	18.885	79 87: 58.997		0 1 9 9 1
ANISOU	16		AASP		1619	2901	6341	790	
ATOM	17	N	BMET		32.709	12.640	58.544		-1022 - 253
ANISOU		N		ī	4552	2218	4435	-105	1580 477
ATOM	18	CA	BMET.		31.874	13.050	57.425		100 4 / /
ANISOU	18	CA		1	4228	4809	6395	580	210 103
MOTA	19	С		1	30.884	14.113	57.894		
ANISOU	19	С		1	5082	3637	5797	282	-909 - 915
ATOM	20	0	BMET	1	30.075	14.599	57.110		
ANISOU	20	0	BMET	1	8292	3208	5525	2071	-656 - 12
ATOM	21	CB	BMET	1	31.131	11.857	56.829		33 14
ANISOU		CB	BMET	1	4866	2613	5114	2013	-122 8 1 8
ATOM	22	CG	BMET	1	29.625	11.840	56.968	0.458	40.28
ANISOU		CG	BMET		4795	5740	4768	230	-751 5 3
ATOM	23	SD	BMET	1	28.761	11.495	55.422		34.23
ANISOU		SD		1	5619	3819	3566	2050	-215 2 0
ATOM	24	CE		1	29.953	12.079	54.222		
ANISOU		CE		1	10672	4519	5420	1149	4083 - 2463
ATOM	25	N	BASP		30.914	14.381	59.194		
ANISOU		N	BASP		4433	3914	5984		-1208 -1385
ATOM	26	CA	BASP		29.979	15.308	59.811	0.732	35.78
ANISOU		CA	BASP		5412	3387	4794		-1050 - 795
ATOM	27	C	BASP		28.536	14.886	59.567		
ANISOU		C	BASP		4876	1624	4771	27 -1	561 1218
ATOM	28	0	BASP		28.181	14.602	58.414	0.732	34.65
ANISOU ATOM		0	BASP		4375	3689	5100	65 -1	485 2 4 7
ANISOU	29	CB	BASP		30.195	16.696	59.181	0.732	37.39
ANISOU	29 30	CB CG	BASP		6632	3351	4222	-1850	869 -1518
ANISOU	30	CG	BASP BASP		29.562	17.730	60.104		
ATOM	31		BASP		3243	3791	4510	-500	
AIOH	JI	ODI	DASP	2	28.866	17.247	61.030	0.732	48.88

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ANISO			1 BAS		6276	4203	8095	-1203 3147 -1901
ATOM ANISO	32	OD	2 BASI	P 2	29.760			5 0.732.3-4,.85
ATOM	U 32 33		2 BASI		2852	3708	6680	-491 444 -1450
ANISO		N N	THR THR	3	27.717		60.606	5 1.000 35.58
ATOM	34	CA		3 3	4586	4123	4811	601 -1628 1516
ANISO		CA		3	26.303 4650	14.433	60.495	1.000 40.48
ATOM	35	C	THR	3	25.382	4555 15.647	6175	371 -911 - 385
ANISO		C	THR	3	4376	4155	6598	1.000 39.82
ATOM	36	0	THR	3	24.150	15.556		320 -3864 -586 1.000 33.55
ANISON		0	THR	3	4668	3107	4972	357 -2748 - 588
ATOM JOSINA	37	CB	THR	3	25.905	13.450		1.000 39.95
ATOM	38	CB	THR 1 THR	3	3787	4004	7387	160 -1209 6 2
ANISOU			1 THR	3 3	26.591	13.851	62.817	1.000 61.83
ATOM	3 9	CG2	2 THR	3	10134 26.399	5882	7476	-4164 -3020 2051
ANISOU	J 39		2 THR	3	4613	12.052 3971	61.2/8	1.000 59.32
MOTA	40	N	THR	4	26.036	16.780	13955	1114 -3135 -198
ANISOU		N	$\mathtt{THR}$	4	4306	4611	3450	1.000 32.55 377 -2166 -217
ATOM	41	CA	THR	4	25.439	18.092	60.393	
ANISOU ATOM	41	CA	THR	4	4275	4229	3358	-81 -1179 9 5
ANISOU		C	THR	4	24.672	18.272	59.090	1.000 30.06
ATOM	43	0	THR THR	4 4	4876	3341	3207	773 -1156 - 204
ANISOU		ŏ	THR	4	25.195 4877	17.935	58.017	1.000 31.64
ATOM	44	CB	THR	4	26.510	3780 19.208	3363	1935 -1255 - 52
ANISOU		СВ	THR	4	2320	4762	5194	1.000 32.31 475 -547 5 9 3
ATOM	45		THR	4	27.324	19.091		475 -547 5 9 3 1.000 3 2 . 3 6
ANISOU ATOM		OG1	THR	4	3705	3955	4635	-79 -797 - 389
ANISOU	46 46	CG2	THR	4	25.852	20.582		1.000 27.22
ATOM		∴N	THR	4	3728	4174	2443	71 304 - 151
ANISOU		N	VAL VAL	5 5	23.464	18.796	59.211	1.000 21.69
ATOM	48	CA	VAL	5	4041 22.690	1985 19.140	2215	-543 -657 1 5 8
ANISOU	48	CA	VAL	5	3675	19.140	2120	1.000 20.42
ATOM	49	С	VAL	5	23.199	20.489		-622 -517 1 0 3 1.000 17.01
ANISOU		C .	VAL	5	2263	1803	2396	-279 -622 8 9
ATOM ANISOU	50	0	VAL	5	23:156	21.449		1.000 21.10
ATOM	50 51	O	VAL	5	3662	1885	2472	-389 -656 1 6
ANISOU	51	CB CB	VAL VAL	5 5	21.204	19.216	58.402	1.000 24.22
ATOM	52		VAL	5	3551	2155	3495	-1045 -396 783
ANISOU	52		VAL	5	20.434 3202	19.700	57.166	1.000 20.14
MOTA	53	CG2	VAL	5	20.701	1779 17.867	2672	-453 10 -226
ANISOU		CG2	VAL	5	5258	2086	3516	1.000 28.58
ATOM	54	N	PRO	6	23.750	20.542	56.300	-1226 431 510 1.000 16.95
ANISOU ATOM		N	PRO	6	2378	1629	2434	29 -594 301
ANISOU	55 55	CA CA	PRO	6	24.354	21.793		1.000 16.90
ATOM	56	CA	PRO PRO	6	1645	1775	3000	6 -445 303
ANISOU		C	PRO	6 6	23.298 1477	22.800	55.383	1.000 15.61
ATOM	57	Õ	PRO	6	22.133	1766	2687	-192 -437 5 4 5
ANISOU	57	Õ	PRO	6	1578	22.432 1761	55.201	1.000 15.75
ATOM	58	CВ	PRO	6	25.216	21.375	2647	-260 -579 5 5 1 000 10 05
ANISOU		CB	PRO	6	2320	1752	34.682	1.000 19.85 50 70 182
ATOM	59	CG	PRO	6	24.632	20.095		1.000 24.76
ANISOU ATOM		CG	PRO	6	3550	2953	2904	-1186 300 -286
ANISOU	60 60	CD	PRO	6	23.926	19.428	55.357	1.000 17.91
ATOM	61	И	PRO THR	6 7	1960	1962	2882	-168 -138 - 44
ANISOU	61	N	THR	7	23.723 1518	24.031	55.156	1.000 14.38
				,	7770	1567	2378	-158 -616 1 0 0

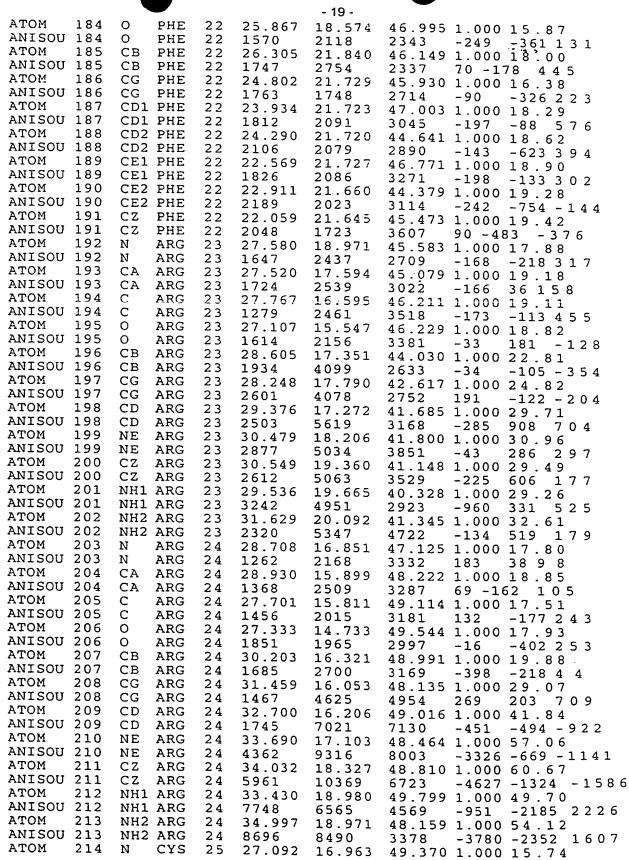
- 15 -MOTA 62 CA THR 7 22.907 25.103 54.610 1.000 14.09 ANISOU 62 CA THR 7 1625 1554 2174 -255 -581 2 2 8 ATOM 63 C THR 7 23.605 25.684 53.374 1.000 14.74 ANISOU 63 C 7 THR 1683 1849 2067 -193 -468 1 2 1 ATOM 7 64 0 THR 24.828 25.894 53.423 1.000 15.95 ANISOU 64 0 7 THR 1752 2137 2171 -378 -457 1 8 5 MOTA 65 CB THR 7 22.795 26.248 55.637 1.000 15.25 ANISOU 65 CB THR 7 1548 56 -124 5 2 1846 2401 OG1 THR ATOM 66 7 22.208 25.717 56.829 1.000 16.91 ANISOU 66 OG1 THR 7 1818 2149 2458 -402 -183 4 7 ATOM 67 CG2 THR 7 21.952 27.387 55.040 1.000 16.09 ANISOU 67 CG2 THR 7 1651 1613 2848 -138 -263 - 25 22.830 25.892 52.325 1.000 15.06 ATOM 68 8 PHE ANISOU 68 Ν PHE 8 1966 1618 2137 -411 -558 2 3 0 ATOM 69 CA PHE 8 23.317 26.545 51.136 1.000 14.76 ANISOU 69 CAPHE 8 1857 1558 2192 -213 -411 2 8 1 7.0 MOTA С PHE 8 22.421 27.728 50.810 1.000 14.94 ANISOU 70 С PHE 8 1907 1421 2347 -275 -357 1 8 1 MOTA 71 0 PHE 8 21.198 27.678 50.995 1.000 16.40 . ANISOU 71 0 PHE 8 1782 1642 2808 -197 -550 3 4 ATOM 72 CB PHE 8 23.242 25.562 49.948 1.000 16.49 ANISOU 72 CB PHE 8 2123 1854 2287 49 - 371 - 1 ATOM 73 CG PHE 8 24.225 24.432 50.027 1.000 14.92 ANISOU 73 PHE CG 8 1710 1824 2135 -197 -365 1 6 3 CD1 PHE 74 ATOM 8 23.822 23.227 50.600 1.000 16.78 ANISOU 74 CD1 PHE 8 1808 1726 -300 -358 1 8 4 2842 CD2 PHE ATOM 75 8 25.539 24.558 49.602 1.000 16.67 CD2 PHE ANISOU 75 8 1705 2130 2500 -310 -361 3 2 1 76 CE1 PHE MOTA 24.702 8 22.183 50.742 1.000 16.74 ANISOU 76 CE1 PHE 8 2035 1966 2359 -4 -99 2 9 5 MOTA 77 CE2 PHE 8 26.420 23.525 49.773 1.000 19.18 ANISOU 77 CE2 PHE 8 1398 2153 3736 -408 -631 187 ATOM 78 26.026 22.336 50.351 1.000 17.90 CZPHE 8 ANISOU 78 CZPHE 8 1849 2003 2948 -119 -376 2 0 ATOM 79 N SER 9 23.023 28.776 50.314 1.000 14.82 ANISOU 79 N 9 SER 2134 1488 2008 -351 -528 3 1 0 ATOM 80 CA SER 9 22.338 29.902 49.715 1.000 15.12 ANISOU 80 CA 9 SER 2037 1259 2449 -357 -571 1 3 4 ATOM 81 С SER 9 21.977 29.607 48.270 1.000 16.19 ANISOU 81 C SER 9 2138 1791 2224 -374 -535 5 4 7 ATOM 9 22.877 29.312 47.473 1.000 17.04 82 0 SER ANISOU 82 0 9 1892 -423 '-544 2 3 2 SER 2191 2393 ATOM 83 CB 9 23.306 31.113 49.696 1.000 18.74 SER ANISOU 83 9 CB SER 2891 1712 2519 -1012 -478 7 1 7 ATOM 9 22.738 32.131 48.853 1.000 20.82 84 OG SER ANISOU 84 OG 9 SER 2866 1569 3477 -662 -854 6 0 7 20.697 ATOM 85 10 N LEU 29.674 47.924 1.000 16.46 ANISOU 85 N LEU 10 2215 1495 2542 -228 -740 - 48 20.345 29.401 46.529 1.000 17.55 MOTA 86 CALEU 10 ANISOU 86 CA LEU 10 2263 2551 1856 -582 -694 3 6 ATOM 87 C 21.079 30.373 LEU 10 45.591 1.000 18.84 С ANISOU 87 LEU 10 2506 1870 2784 -596 -830 3 5 7 MOTA 88 0 21.573 30.025 LEU 10 44.520 1.000 20.19 ANISOU 88 0 LEU 2705 10 2263 2704 -524 -663 5 0 8 ATOM 89 CB 18.844 29.559 46.327 1.000 18.87 LEU 10 ANISOU 89 CB LEU 10 2302 2516 2354 -288 -715 2 8 0 18.355 29.333 ATOM 90 CG LEU 10 44.895 1.000 18.28 ANISOU 90 CG LEU 10 2182 2172 2591 -668 -677 - 301 91 18.708 27.955 44.397 1.000 22.45 ATOM CD1 LEU 10 ANISOU 91 CD1 LEU 10 3418 3089 -308 -537 1 7 2024 ATOM 92 CD2 LEU 10 16.852 29.603 44.869 1.000 21.93

						- 16 -			
ANISOU			LEU	10	2250	2658	3424	-504	-1139 7 5
ATOM ANISOU	93 193	N N	ALA	11	21.154	31.638	46.037		). 2.0, ., 0 5
ATOM	94	CA	ALA ALA	11 11	2862 21.810	1780	2977	-595	-1279 472
ANISOU		CA	ALA	11	3160	32.647 1670	45.202	1.000	24.24
ATOM	95	С	ALA	11	23.285	32.309		-455 1 000	-979 8 9 1 9 2 1 . 0 6
ANISOU		C	ALA	11	3128	1937	2937	-644	-1016 431
ATOM ANISOU	96	0	ALA	11	23.819	32.447	43.829	1.000	26.29
ATOM	97	CB	ALA ALA	11 11	3569	3261	3158	-1628	-923 1137
ANISOU		CB	ALA	11	21.752 3740	33.989 1692	45.953		24.29
ATOM	98	N	GLU	12	23.953	31.844	3797 46 005	-461 1 000	-216 9 9 6 20.65
ANISOU ATOM		N	GLU	12	2829	1975	3044	-828	-930 6 7 4
ANISOU	99	CA CA	GLU	12	25.354	31.463	45.862	1.000	21.19
ATOM	100	CA	GLU GLU	12 12	3036 25.483	2400	2615	-506	-715 5 9 8
ANISOU		č	GLU	12	3894	30.277 2179	44.920 2117	1.000	21.56
MOTA	101	0	GLU	12	26.375	30.215	44 069	-702	-206 9 8 8 21.98
ANISOU		.0	GLU	12	3463	2917	1971	-1144	-488 6 1 8
ATOM ANISOU	102 102	CB	GLU	12	26.032	31.170	47.204	1.000	20.27
ATOM	103	CB CG	GLU GLU	12	2874	2192	2636	-221	-624 5 0 1
ANISOU		CG	GLU	12 12	26.156 2889	32.451 2316	48.032	1.000	20.54
MOTA	104	CD	GLU	12	26.787	32.279	2598 49.389	-344	-516 4 0 6
ANISOU		CD	GLU	12	3146	2542	2619		21.86 -612 7 9 9
ATOM ANISOU	105 105		GLU	12	27.068	31.149	49.803	1.000	24.98
ATOM	106		GLU GLU	12 12	3642	2681	3169	-1348	-1088 1134
ANISOU		OE2	GLU	12	26.819 5881	33.305 2966	50.092	1.000	33.52
ATOM	107	N	LEU	13	24.600	29.295	3888 45.060	-1119	-2251 4 6
ANISOU	107	N	LEU	13	2567	2345	2275	-351	-390 3 8 2
ATOM ANISOU	108 108	CA	LEU	13	24.645	28.117	44.174	1.000	18.61
ATOM.	108	CA C	LEU LEU	13 13	2575	2347	2149	-209	270 406
ANISOU	109	C	LEU	13	24.432 3558	28.566 2367	42.738		
ATOM	110	0	LEU	13	25.102	28.095	2206 41.824	-709 1 000	-41 5 2 6
ANISOU		0	LEU	13	3827	3216	1981	-823	-117 1 9 0
ATOM ANISOU	111 111	CB	LEU	13	23.541	27.137	44.562		18.97
ATOM	112	CB CG	LEU LEU	13 13	2982	2243	1984	-462	-145 4 4 0
ANISOU	112	CG	LEU	13	23.773 2313	26.344 2322	45.860	1.000	18.57
MOTA	113	CD1	LEU	13	22.526	25.480	2422 46.070	-467	-362 7 4 5
ANISOU	113	CD1		13	2769	2266	2845	-789	-142 5 9 4
ATOM ANISOU	114	CD2	LEU	13	25.023	25.473	45.858	1.000	19.80
ATOM	115	CD2	GLN	13	2709	2229	2585	-244	-509 - 107
ANISOU	115	N	GLN	14 14	23.544 3596	29.508 2139	42.478	1.000	
ATOM	116	CA	GLN	14	23.284	29.978	2635 41.104	-960	-903 3 7 9
ANISOU		CA	GLN	14	3010	3335	2694	-992	-816 6 4 8
ATOM ANISOU	117	C	GLN	14	24.481	30.712	40.509	1.000	25.44
ATOM	117 118	C 0	GLN GLN	14 14	3360	3427	2881	-1070	-382 4 8 7
ANISOU	118	ŏ	GLN	14	24.655 3836	30.829 4657	39.288	1.000	30.04
ATOM	119	ČВ	GLN	14	22.064	30.906	2922 41.131	-1208	-427 8 9 8
ANISOU	119	CB	GLN	14	3133	3630	3222	-760	-863 9 3 8
ATOM ANISOU	120	CG	GLN	14	20.772	30.111	41.355	1.000	23.26
ATOM	121	CG CD	GLN GLN	14	3106	2319	3413	-299	-577 5 1 4
ANISOU	121	CD	GLN	14 14	19.586 3384	31.020	41.631		
ATOM	122	OE1		14	19.734	2462 32.104	3155 42.160	-317	-393 - 196
ANISOU	122	OE1		14	4973	2619	3175	-183	28.34 -732 - 408
							<del></del>	_ ~ ~ ~	132 - 400



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ATOM	123	NE2	GLN	14	18.398	30.513	41.349	1.000	23.60
ANISOU	123	NE2	GLN	14	3058	2969			
MOTA	124	N	GLN	15	25.309	31.243	41.395	1.000	54 2 4 5 25:00
ANISOU		N	GLN	15	3078	3281	3140		-394 5 7 5
ATOM	125	CA	GLN	15	26.530	31.936	40.945		
ANISOU	125	CA	GLN	15	2947	3560	2631	-866	-98 655
ATOM	126	С	GLN	15	27.650	30.920	40.707	1.000	
ANISOU	126	С	GLN	15	3810	3951	2139	-345	406 668
MOTA	127	0	GLN	15	28.756	31.284	40.302		
ANISOU	127	0	GLN	15	4294	4851	4476	102	1871 1192
ATOM	128	CB	GLN	15	27.018	32.918	42.009	1.000	25.90
ANISOU		CB	GLN	15	3055	3037	3748		-109 3 6 4
MOTA	129	CG	GLN	15	26.103	34.092	42.219	1.000	31.24
ANISOU	129	CG	GLN	15	4562	2577	4731	-806	962 1054
MOTA	130	CD	GLN	15	26.503	35.022	43.348	1.000	59.75
ANISOU		CD	GLN	15	9927	2475	10301		-14 -1904
ATOM	131	OE1	GLN	15	27.634	35.031	43.840	1.000	81.81
ANISOU		OE1	GLN	15	15059	3931	12094	-944	
ATOM	132		GLN	15	25.539	35.841	43.767	1.000	91.46
ANISOU		NE2	GLN	15	14070	4846	15833	-923	3672 - 4850
ATOM	133	N	GLY	16	27.379	29.643	40.969		29.90
ANISOU		N	GLY	16	4634	3820	2907	-239	22 7 8 7
ATOM	134	CA	GLY	16	28.410	28.649	40.699		
ANISOU		CA	GLY	16	4466	3629	2833	-709	461 250
ATOM	135	C	GLY	16	29.339	28.473	41.878		
ANISOU		C	GLY	16	3816	3779	2891	-616	
ATOM	136	0	GLY	16	30.398	27.867	41.725		
ANISOU		0	GLY	16	3386	4758	3814	-899	1243 1023
ATOM	137	N	LEU	17	28.960	28.898	43.083		
ANISOU ATOM	137	N	LEU	17	3295	3636	2950	-721	162 743
ANISOU		CA CA	LEU	17 17	29.776	28.666	44.257		23.96
ATOM	139	CA	LEU LEU	17	2700	3032	3372	-601	100 673
ANISOU		C	LEU	17	29.462 2222	27.338	44.932		
ATOM	140	0	LEU	17	28.389	2763 26.780	2733	-252	611 261
ANISOU		Ö	LEU	17	2347	3134	44.789 3308		23.13 263 859
ATOM	141	CB	LEU	17	29.645	29.806	45.286	-443	
ANISOU		CB	LEU	17	2886	2933	4035		-405 2 5 4
ATOM	142	CG	LEU	17	29.962	31.209	44.716		
ANISOU		ĊĞ	LEU	17	3741	2948	5308	-523	
ATOM	143		LEU	17	29.550	32.358	45.615		
ANISOU			LEU	17	5221	2887	4066	-1269	
ATOM					31.458	31.278	44.416	1.000	38.11
ANISOU			LEU	17	3828	5491	5160		954 232
ATOM	145	N	HIS	18	30.441	26.822	45.681		
ANISOU	145	N	HIS	18	2600	3067	2877	-662	42 4 4 9
ATOM	146	CA	HIS	18	30.289	25.644	46.537		
UOZINA	146	CA	HIS	18	2378	2809	2996	-432	201 313
MOTA	147	С	HIS	18	29.908	24.376	45.790		
ANISOU	147	С	HIS	18	2256	3245	3148	-1009	
MOTA	148	0	HIS	18	29.147	23.565	46.331	1.000	22.60
ANISOU	148	0	HIS	18	2008	3064	3516	-629	
$\mathtt{MOTA}$	149	CB	HIS	18	29.224	25.872	47.618	1.000	22.81
ANISOU		СВ	HIS	18	2514	2879	3272	-526	450 421
MOTA	150	CG	HIS	18	29.320	27.248	48.217		21.70
ANISOU		CG	HIS	18	2 <b>7</b> 97	3038	2411	-149	39 5 0 3
MOTA	151		HIS	18	30.438	27.773			25.01
ANISOU			HIS	18	3714	3505	2284	-207	-629 1 4 9
ATOM	152		HIS	18	28.370	28.216	48.269		
ANISOU			HIS	18	3244	3278	2957		4 2 7 5
MOTA	153	CE1	HIS	18	30.197	28.982	49.223	1.000	29.26

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ANISOU	J 153	<u></u>	1 1170			- 18 -			
ATOM	154	CE.	HIS	18	4603	3396	3118	-388	-335 2 7
ANISOU	154	NEA	2 HIS	18	28.937	29.271	48.919	1.000	.27, 24
ATOM	155	N E 2	2 HIS	18	4582	3137	2632	2 22	4 3 6 5
ANISOU		N	GLN	19	30.269	24.270	44.521	1.000	22.74
ATOM	156		GLN	19	2724	3094	2822	-511	-123 4 2 3
ANISOU		CA	GLN	19	29.806	23.113	43.730	1.000	23.85
ATOM	157	CA	GLN	19	3129	2668	3263	148	63 8 9
ANISOU		C	GLN	19	30.271	21.760	44.221	1.000	22.77
ATOM	158	0	GLN	19	2532	3026	3095	-502	-574 7 7 g
ANISOU		0	GLN GLN	19	29.480	20.801	44.259	1.000	21.99
ATOM	159	CB	GLN	19	1869	2911	3574	-187	0 558
ANISOU		CB	GLN	19 19	30.227	23.322	42.276	1.000	27.66
ATOM	160	CG	GLN	19	5043 29.397	2519	2947	29 -3	39 458
ANISOU		CG	GLN	19	3289	24.333	41.523	1.000	26.21
ATOM	161	CD	GLN	19	27.917	3163	3508	299	171 437
ANISOU		CD	GLN	19	3403	24.368 4411	41.862	1.000	
ATOM	162		GLN	19	27.154	23.604	4521	-986	535 654
ANISOU	162	OE1	GLN	19	3996	4238	41.277	1.000	
ATOM	163	NE2	GLN	19	27.511	25.212	6845	-262	-2770 1829
ANISOU	163		GLN	19	3803	6153	42.811 6212	1.000	
$\mathtt{ATOM}$	164	N	ASP	20	31.526	21.572	0212	81 19	44 1 1
ANISOU		N	ASP	20	2073	3400	44.631 3123	1.000	
ATOM	165	CA	ASP	20	31.926	20.292		-414	95 7 0 8
ANISOU		CA	ASP	20	1869	3674	45.225 3235	1.000	23.10
ATOM	166	С	ASP	20	31.190	20.042	46.546	1 000	6704
ANISOU		С	ASP	20	1775	2963	2873	-280	-143 4 9 3
ATOM	167	0	ASP	20	30.772	18.899	46.768	1 000	-143 4 9 3
ANISOU		0	ASP	20	1429	2884	3848	-311	225 224
ATOM	168	CB	ASP	20	33.414	20.268	45.521	1 000	223 224
ANISOU	168	CB	ASP	20	1835	4546	4130	-16	207 881
ATOM ANISOU	169	. CG	ASP	20	34.298	20.206	44.291	1.000	39.35
ATOM		CG	ASP	20	2355	6893	5705	-654	1323 - 1915
ANISOU	170 170	ODI	ASP	20	33.870	19.914	43.153	1.000	35.78
ATOM	171		ASP	20	3152.	5452	4992	-741	1508 - 797
ANISOU	171	002	ASP ASP	20	35.508	20.433	44.467	1.000	45.22
ATOM	172	N N		20	2201	8705	6277	-589	1088 - 87
ANISOU		N	GLU GLU	21	31.046	21.053	47.404	1.000	20.01
ATOM	173	CA	GLU	21 21	1574	2935	3093	-412	-241 3 6 7
ANISOU	173	CA	GLU	21	30.323 1412	20.811	48.665	1.000	
	174		GLU			2956	2838	-481	-464 1 1 8
ANISOU	174	Č	GLU	21	1386		48.402		
ATOM	175	Ō	GLU	21	28.290	2342	3050	-307	-395 2 3 4
ANISOU	175	0	GLU	21	1671	19.602 2286	49.054	1.000	
ATOM	176	СВ	GLU	21	30.415	22.058	3057	-419	-351 1 1 6
ANISOU	176	CВ	GLU	21	1646	2821	49.563		20.10
ATOM	177	CG	GLU	21	31.893	22.322	3170	-514	-499 1 2 7
ANISOU		CG	GLU	21	1682	3568	49.918 3912	7.000	24.11
ATOM	178	CD	GLU	21	32.574	23.380	49.081	-766	-326 - 711
ANISOU		CD	GLU	21	1330	4241	5713	-752	
ATOM	179	OE1		21	32.249	23.594	47.887	1 000	-666 5 2 1
ANISOU		OE1	GLU	21	2623	4054	6677	-1336	-1741 1977
ATOM	180	OE2	GLU	21	33.483	24.007	49.678	1 000	-1/41 19//
ANISOU		OE2		21	3681	4425	6860	-2089	-1618 647
ATOM	181	N	PHE	22	28.231	21.048	47.395	1.000	17 30
ANISOU		N	PHE	22	1540	2352	2680	-243	-446 - 79
ATOM	182	CA	PHE	22	26.851	20.761	47.071	1.000	17.13
ANISOU ATOM		CA	PHE	22	1534	2166	2807	-235	-396 3 7 4
ANISOU	183	C	PHE	22	26.733	19.329			17.41
-111200	102	С	PHE	22	1688	2500	2427	-502	-334 1 0 4



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ANISO			CYS			1969	2574	-16	203	
ATOM	215	CA			25.884	16.921	50.22		- 393 - 1.6, 3:	- 33
ANISO ATOM						1954	2756	-95	-317 -	7 0 0
ANISO	216	_	CYS			16.068		7 1 000	15.7	. 3 0 0
ATOM	U 216 217		CYS	25		1699	2648	-114	-432 e	) :
ANISO		•	CYS	25	24.124		50.15	5 1.000	15.89	2
ATOM	218	O CB	CYS CYS	25	1453	1801	2783	-88	-469 2	5.2
ANISO		CB	CYS	25	25.367		50.424	1 1.000	15.93	3 2
ATOM	219	SG	CYS	25 25	1644	1779	2629	-49	-261 -	3 0
ANISO		SG	CYS	25	23.700 1742	18.417	51.184	1 1.000	17.82	!
ATOM	220	N	LEU	26	24.623	1825	3202	-122	-33 _	5 5
ANISO		N	LEU	26	1449	16.308 1843	48.250	1.000	15.25	
ATOM	221	CA	LEU	26	23.560	15.590	2504	-54	-263 -	142
ANISO		CA	LEU	26	1616	1739	2580	-86	15.62	
ATOM	222	C	LEU	26	23.763	14.085		1 000	-453 4 15.18	8
ANISOU ATOM		C	LEU	26	1697	1764	2306	-113	-479 6	
ANISOU	223	0	LEU	26	22.819	13.345	47.771	1 000	16.96	
ATOM	224	O CB	LEU	26	1797	1725	2920	-234	-664 -	3 0 0
ANISOU		CB	LEU LEU	26	23.526	16.068	46.066	1.000	16.02	300
ATOM	225	CG	LEU	26 26	1811	1645	2633	-191	-483 1	2 2
ANISOU		CG	LEU	26	23.057 1762	17.510	45.864	1.000	15.69	
ATOM	226		LEU	26	23.252	1716	2485	-6 -1	579	
ANISOU	226	CD1	LEU	26	1750	17.880 2360	44.405		17.48	
ATOM	227	CD2	LEU	26	21.584	17.680	2532	-17	-130 4	6 5
ANISOU			LEU	26	1655	2188	46.290 2660	1.000		_
ATOM	228	N	ARG	27	25.027	13.648	47.494	-29	-75 <u>1</u>	6 8
ANISOU ATOM		N	ARG	27	1870	1818	2871	155	17.26	
ANISOU	229	CA	ARG	27	25.295	12.205	47.372	1.000	-326 1 18 75	4 0
ATOM	230	CA C	ARG	27	2108	1845	3170	270	-955 1	0.2
ANISOU		C	ARG ARG	27 27	25.240	11.599	48.744	1.000	17.95	0 2
ATOM	231	ŏ	ARG	27	1667 24.777	1801	3351	159	-897 2	19
ANISOU	231	ŏ	ARG	27	24.777	10.454	48.913	1.000	20.99	
ATOM	232	ČВ	ARG	27	26.641	1793	4026	-43	-3601	6 8
ANISOU	232	CB	ARG	27	2815	12.008 2034	46.670	1.000	21.35	
ATOM	233	N	ASP	28	25.827	12.293	3264	622	-377 - 3	129
ANISOU		N	ASP	28	1487	2004	49.723 2856			_
ATOM	234	CA	ASP	28	26.034	11.672	51.026	178	-328 6	/
ANISOU ATOM	234	CA	ASP	28	1613	2095	2931	107	-301 1	2 7
ANISOU	235	C	ASP	28	24.872	11.866	51.990	1.000	17 22	2 /
ATOM	236	0	ASP ASP	28	1414	2264	2863	223	-447 4	7 1
ANISOU	236	Ö	ASP	28 28	24.816	11.081	52.937	1.000	17.62	-
ATOM	237	СB	ASP	28	1932 27.306	2139	2624	150	-565 3	2 7
ANISOU	237	CB	ASP	28	1581	12.237	51.657	1.000	22.17	
ATOM	238	CG	ASP	28	28.590	3894 11.906	2948	-272	-467 5	59
ANISOU		CG	ASP	28	1596	3323	50.941			
ATOM	239	OD1		28	28.572	10.905	4472	236	-288 6	48
ANISOU		OD1		28	2317	3071	50.199 5084			
ATOM ANISOU	240	OD2	ASP	28	29.573	12.617	51.251	808	-284 5	12
ATOM		OD2		28	1584	4343	6261	-144	-470 4 :	1 6
ANISOU	241	N	LYS	29	24.098	12.942	51.821	1.000	15.57	
ATOM	241		LYS	29	1475	1814	2627	5 -30	3 178	
	242		LYS LYS	29	23.048	13.305	52.778	1.000	15.13	
ATOM	243		LYS	29 29	1584	1999	2165	-68	-500 - 9	9 6
NOSINA	243		LYS	29	21.686 1496	13.500	52.118	1.000	14.56	
ATOM	244		LYS	29	20.688	1352 12.985	2686	77 -45	2 106	
ANISOU	244		LYS	29	1627	1876	52.635	1.000	16.21	
			_		_ 00 /	T010	2657	-177	-315 -	5



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MOTA	245	CB	LYS	29	23.431	14.563	53 574	1.000 16.09
ANISOU		СВ	LYS	29	1666	1672	2777	3 -642 25
ATOM	246	CG	LYS	29	24.776	14.421		1 000 17 (0
							54.292	1.000 17.68
ANISOU		CG	LYS	29	2192	1918	2606	71144 1 4 1
ATOM	247	CD	LYS	29	25.161	15.647	55.096	1.000 20.71
ANISOU	247	CD	LYS	29	2675	2044	3151	-35 -1518 4 1
ATOM	248	CE	LYS	29	26.498	15.331	55.844	1.000 22.24
ANISOU		CE	LYS	29	2203	2714	3535	
ATOM	249	ΝZ	LYS	29	26.955	16.594		142 -1369 - 685
							56.492	1.000 32.67
NISOU		ΝZ	LYS	29	3199	3381	5831	-502 -2085 -1260
ATOM	250	N	$\mathtt{GLY}$	3 0	21.604	14.198	50.993	1.000 14.09
UOZINA	250	N	$\mathtt{GLY}$	3 0	1552	1461	2340	135 -455 -100
ATOM	251	CA	GLY	30	20.358	14.373	50.250	1.000 14.09
ANISOU	251	CA	GLY	30	1428	1561	2365	92 -342 - 97
ATOM	252	С	GLY	3 0	19.372	15.284		
ANISOU		Č	GLY	30	1423	1192		
							2059	-95 -275 9 4
ATOM	253	0	GLY	30	18.168	15.223		1.000 14.58
ANISOU		Ο.	GLY	30	1435	1689	2415	52 -476 -121
MOTA	254	N	LEU	31	19.884	16.146	51.823	1.000 13.93
ANISOU	254	N	LEU	31	1472	1479	2343	-182 -248 -181
ATOM	255	CA	LEU	31	19.012	17.114	52 511	1.000 14.44
ANISOU		CA	LEU	31	1534	1457	2495	-235 -55 -246
ATOM	256	C	LEU	31	19.894	18.286		1 000 15 00
							52.942	1.000 15.08
ANISOU		C	LEU	31	1411	1535	2784	-177 -326 -314
ATOM	257	0	LEU	31	21.113	18.136		1.000 15.64
ANISOU		0	LEU	31	1468	1664	2812	-169 -328 - 67
ATOM	258	CB	LEU	31	18.222	16.560	53.694	1.000 16.76
ANISOU	258	CB	LEU	31	2192	1664	2511	-367 128 -213
ATOM	259	CG	LEU	31	18.883	16.517	55.039	1.000 20.16
ANISOU		CG	LEU	31	2435	2485	2739	
ATOM								-289 -141 4 4 5
	260	CD1		31	17.977	16.145		1.000 26.49
ANISOU		CD1		31	2253	5076	2738	-508 -341 9 6 9
ATOM	261		LEU	31	20.052	15.526	55.032	1.000 24.73
ANISOU	261	CD2	LEU	31	4192	2967	2237	1001 153 610
ATOM	262	N	PHE	32	19.289	19.462		1.000 14.11
UOSINA	262	N	PHE	32	1569	1457	2335	-231 -179 - 207
ATOM	263	CA	PHE	32	20.020	20.697		1.000 13.56
ANISOU		CA	PHE	32				
					1447	1389	2317	-225 -137 1 4
ATOM	264	C	PHE	32	18.976	21.777		1.000 13.72
ANISOU		С	PHE	32	1411	1439	2365	-218 -421 -142
MOTA	265	0	PHE	32	17.889	21.711	53.118	1.000 15.50
ANISOU	265	0	PHE	32	1392	1862	2634	-175 -436 -389
MOTA	266	CB	PHE	32	20.958			1.000 15.01
ANISOU		СB	PHE	32	1379	2201	2125	-305 -342 2 3 1
ATOM	267	CG	PHE	32	20.381			
ANISOU						21.156		1.000 14.60
		CG	PHE	32	1649	1662	2237	-193 -429 1 1 8
ATOM	268		PHE	32	20.326	19.986	50.148	
ANISOU	268	CD1	PHE	32	1328	1688	2504	-156 -507 1 5
ATOM	269	CD2	PHE	32	19.831	22.345	50.396	1.000 13.66
ANISOU	269	CD2	PHE	32	1320	1678	2191	-179 -309 1 6 6
ATOM	270		PHE	32	19.742	20.033		1.000 14.26
ANISOU			PHE	32	1507			
						1655	2256	-346 -271 1 9 9
ATOM	271		PHE	32	19.267	22.348		1.000 15.49
ANISOU			PHE	32	1681	1932	2272	72 -504 -126
ATOM	272	CZ	PHE	32	19.177	21.184	48.385	1.000 15.25
ANISOU	272	CZ	PHE	32	1979	1700	2117	-185 -295 1 6 8
ATOM	273	N	TYR	3 3	19.376	22.785		1.000 14.44
ANISOU		N	TYR	33	1813	1302	2372	
ATOM	274	CA	TYR	33				
					18.616	24.023		1.000 14.32
ANISOU		CA	TYR	33	1764	1415	2261	-143 -295 -111
ATOM	275	С	TYR	33	19.039	24.929	53.364	1.000 13.70

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ANISO		-	TYR	33	1479	1565	2161	7.0	
ATOM	276		TYR		20.158	24.871		-79	
ANISO		-	TYR		1370	1524	52.85 2912		0 15 28
ATOM	277		TYR		18.874	24.734	2912	-190	-420 2 6 3
ANISO					1648	1717		3 1.00	0 14 . 47
ATOM	278	CG	TYR		18.231	24.046	2133	-197	
ANISO	U 278	CG		_	2131	1537			0 15.71
$\mathtt{ATOM}$	279	CD	1 TYR	33	16.938	24.390	2302	-339	-109 - 136
ANISO	U 279	CD	1 TYR	33	2478	1967	3/.45.	3 1.000	0 17.41
ATOM	280	CD	2 TYR	33	18.912	23.116	2172	-154	246 - 249
ANISO	J 280	CD.	2 TYR	3 3	2901	2070	57.799		0 19.58
ATOM	281	CE	1 TYR	3 3	16.354	23.758	2468	144	115 192
ANISO		CE.	1 TYR	3 3	3138	1948	2581	1.000	20.18
ATOM	282	CE:	2 TYR	33	18.368	22.475	58.90(	26 74	10 - 102
ANISO		CE:	2 TYR	33	3571	2480	2118		21.50
ATOM	283	CZ	TYR	3 3	17.081	22.821	59.263	340	196 122
ANISO	_	CZ	TYR	33	4140	1772	2454	_	22.02
ATOM	284	OH	TYR	33	16.541	22.194	4434 60 355	471	1035 - 105
ANISOU		ОН	TYR	33	5088	2809	3329	1.000	29.55
ATOM	285	N	LEU	34	18.076	25.709	52.878	377	1512 7 2 8
ANISOU		N	LEU	34	1496	1533	2396		14.28
ATOM	286	CA	LEU	34	18.278	26.620	2330 51 756	-80	-517 - 17
ANISOU		CA	LEU	34	1830	1452	2425	1.000	15.02
ATOM	287	С	LEU	34	17.871	28.039		-126	-580 2 0
ANISOU		С	LEU	34	1703	1575	2217	1.000	14.46
ATOM	288	0	LEU	34	16.716	28.289	52.492	-146	-241 - 7
ANISOU		0	LEU	34	1663	1852	2923	-75	16.95
ATOM	289	CB	LEU	34	17.389	26.127	50.598		-186 - 64 16.54
ANISOU		CB	LEU	34	2355	1485	2444	-212	
ATOM	290	CG	LEU	34	17.633	26.800	49.249	1 000	-749 2 5 15.65
ANISOU ATOM		CG	LEU	34	2010	1567	2371	-7 -6	
ANISOU	291	CD1	LEU	34	18.977	26.422	48.664	1 000	33 - 63 20.14
ANISOU		CD1	LEU	34	1919	2018	3717	-225	-171 2 6 0
ANISOU	292	CD2	LEU	34	16.490	26.535		1 000	17.29
ATOM			LEU	34	2152	1824	2592	-425	-819 2 1 4
ANISOU	293	N	THR	35	18.842	28.944	52.065		15.48
ATOM	293	N	THR	35	1817	1532	2534	-230	-200 1 3
ANISOU		CA	THR	35	18.587	30.362	52.324	1.000	17.02
ATOM	295	CA	THR	35	2149	1537	2781	-206	-827 - 196
ANISOU	295	С	THR	35	18.491	31.127	51.010	1.000	17.04
ATOM	296	C	THR	35	1895	1693	2887	-149	-882 - 44
ANISOU		0	THR	35	18.765	30.572		1.000	17.01
ATOM	297	0	THR	35	1880	1692	2893	-262	-458 1 4 4
ANISOU	297	CB CB	THR	35	19.772	30.917	53.180	1.000	17.79
ATOM	298		THR	35	2018	1942	2800	-87	-854 - 200
ANISOU	298	061	THR	35	20.986	30.673	52.474	1.000	21.10
ATOM	299	CC3	THR THR	35	2110	2035	3873	-253	-364 - 402
ANISOU	299	CG2	THR	35	19.847	30.331	54.567	1.000	20.44
ATOM	300	N N		35	2600	2194	2971	228	-1113 5 9
ANISOU	300		ASP	36	18.186	32.407	51.059	1.000	18.62
ATOM	301	N CA	ASP	36	2287	1747	3040	-187	-316 1 4 9
ANISOU	301	CA	ASP	36	18.240	33.300	49.884	1.000	20.75
ATOM	302	CA	ASP	36	2678	1722	3483	-632	-508 3 7 4
ANISOU	302	C	ASP ASP	36	17.474	32.711	48.703		20.05
ATOM	303	0	ASP	36	2104	1929	3586	198	-928 4 8 9
ANISOU	303	0	ASP	36	17.929	32.685	47.540	1.000	21.06
ATOM	304	СВ	ASP	36	2593	1749	3662	-496	-756 1 3 1
ANISOU	304	CB	ASP	36	19.703	33.561	49.500	1.000	22.21
ATOM	305	CG	ASP	36	2666	2366	3406	-876	-755 8 0 7
ANISOU	305	CG	ASP	3 6 3 6	20.588	34.192	50.551	1.000	23.05
	300	- 0	ASF	3 6	2537	1818	4402	-175	-833 - 208

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ATOM	306	OD1	ASP	36	20.061	34.886	51.457	1.000	26.16
ANISOU	306	ODl	ASP	36	2981	2100			777 - 381
ATOM	307	OD2		36	21.824	33.982	50.528	1.000	24.87
ANISOU	307	OD2	ASP	36	2532	1994			-950 -628
ATOM	308	N	CYS	37	16.282	32.196	48.971		
ANISOU	308	N	CYS	37	2135	1711	3849		-638 - 263
ATOM	309	CA	CYS	37	15.463	31.587	47.902		
ANISOU	309	CA	CYS	37	2390	1478	3839		-799 -138
ATOM	310	С	CYS	37	14.078	32.183			
ANISOU	310	С	CYS	37	2374	1724	3463		-711 - 7 4
MOTA	311	0	CYS	37	13.176	31.629	47.156		
ANISOU		0	CYS	37	2569	1984	4091	-12	-1108 1 5
$\mathtt{ATOM}$	312	СВ	CYS	37	15.359	30.061	48.083		
ANISOU	312	CB	CYS	37	2739	1454	4247	194	-477 -115
MOTA	313	SG	CYS	37	14.500	29.595	49.596	1.000	22.84
ANISOU		SG	CYS		2854	1884	3942		-922 1 4 1
$\mathtt{ATOM}$	314	N	$\mathtt{GLY}$	38	13.855	33.390			20.85
ANISOU		N	GLY	38	2353	1638	3933		-375 - 42
ATOM	315	CA	$\mathtt{GLY}$	38	12.570	34.044			
ANISOU		CA	$\mathtt{GLY}$	38	2233	1874	4790	255	-292 1 6 5
MOTA	316	С	GLY	38	11.534	33.619			
ANISOU		С	$\mathtt{GLY}$	38	2577	2045	4228		-136 -601
MOTA	317	0	GLY	38	10.400	34.091			
ANISOU		0	GLY	38	2529	3424	3765	214	-96 -264
ATOM	318	N	LEU	39	11.894	32.836			
ANISOU		N	LEU	39	2310	2980	4037	119	-46 -364
ATOM	319	CA	LEU	39	10.938	32.331	51.195		
ANISOU		CA	LEU	39	2637	2964	3684	-105	175 - 946
ATOM	320	C	LEU	39	11.107	32.885	52.593		
ANISOU		C	LEU	39	5341	4215	3898	-796	
ATOM	321	0	LEU	39	11.784	32.313	53.441		
ANISOU ATOM	322	O CB	LEU LEU	39 39	7338 10.850	4986 30.810	4171 51.206		-1333 - 303
ANISOU		CB	LEU	39	4244	2940	2879		) - 261
ATOM	323	CG	LEU	39	10.404		49.921		
ANISOU		CG	LEU	39	4834	2452		258	-1618 - 474
ATOM	324		LEU	39	10.683	28.595	49.972	1 000	
ANISOU			LEU	39	3351	2597	3468	424	-707 - 118
ATOM	325		LEU	39	8.940	30.407			
ANISOU			LEU	39	4828	2118	3503	860	-860 - 323
ATOM	326	N	THR	40	10.365	33.957	52.882		
ANISOU		N	THR	40	7392	4849	5077		2852 - 1993
	327	CA		40		34.661			
ANISOU		CA	THR	40	4224	3732	4393	999	961 - 558
MOTA	328	С	THR	40	9.700	34.177	55.248		29.68
ANISOU	328	С	THR	40	3175	4204	3898	-116	294 -1630
ATOM	329	0	THR	40	8.653	33.556			39.75
ANISOU	329	0	THR	40	3930	5847	5326	-1079	-301 -1653
MOTA	330	СВ	THR	40	10.641	36.183	53.997	1.000	56.31
ANISOU		СB	THR	40	10586	3758	7052		1006 - 992
ATOM	331		THR	40	11.545	36.606		1.000	68.39
ANISOU			THR	40	7379	3900	14707		3617 - 246
ATOM	332		THR	40	11.214	36.837			70.22
ANISOU			THR	40	8265	5228	13188	1389	
ATOM	333	N	ASP	41	10.191	34.302			33.20
ANISOU		N	ASP	41		5223	3810	-203	307 -1779
ATOM	334	CA	ASP	41	9.329	33.943			27.51
ANISOU		CA	ASP	41	2705	3858	3891	91 -2	
ATOM	335	C	ASP	41	8.107	34.861			33.43
ANISOU		C	ASP	41	3131	3064	6508		7 - 1307
MOTA	336	0	ASP	41	7.034	34.469	58.101	. т.ооо	30.76

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ANISC	U 336		ASP		2690	3223	5774	• • •
ATOM	337				10.113	34.135		141 -149 - 969 5 1.000 33,51
ANISO ATOM					4853	4026	3852	-1222 -698 -938
	338 U 338	CG CG				33.351	60.039	9 1.000 33.37
ATOM	339		ASP 1 ASP		3324	5291	4065	-739 -501 -571
ANISO	บ 339		l ASP		9.152 4040	32.164		1.000 34.95
ATOM	340	OD:	2 ASP	41	9.395	4681 33.904	4557	-380 824 - 9.2
ANISO		OD:	2 ASP	41	18972	10427	61.161 3567	1.000 86.76
ATOM	341	N	THR	42	8.272	36.089	57.205	-10425 588 -1858
ANISO ATOM	341	N	THR	42	3217	3695	5516	1.000 32.71 9 -58 - 586
ANISO		CA CA	THR THR	42	7.198	37.074	57.221	1.000 38.48
ATOM	343	C	THR	42 42	4747 6.005	4161	2/11	1067 -861 - 630
ANISO	J 343	Ċ	THR	42	3333	36.640 4044		1.000 35.83
ATOM	344	0	THR	42	4.877	36.606	6237	1136 157 -1162
ANISO		0	THR	42	4048	3603	7128	1.000 38.90 1186 1059 1224
ATOM ANISO	345 345	CB	THR	42	7.751	38.449		1186 1059 1224 1.000 37.05
ATOM	346	CB OG1	THR THR	42	4526	3763	5/88	1021 -677 -1532
ANISOU	J 346	061	THR	42 42	8.831	38.301	55.889	1.000 98.08
ATOM	347	CG2	THR	42	16381 8.358	13757	7127	-3208 7500 - 231g
ANISOU		CG2	THR	42	6097	39.113 3613	58.047	1.000 36.08
ATOM	348	N	GLU	43	6.259	36.184	3997 55.173	886 -1119 269
ANISOU ATOM	-	N	GLU	43	4208	3312	5642	1.000 34.64 656 -275 -698
ANISOU	349	CA CA	GLU	43	5.391	35.557	54.192	1.000 32.98
ATOM	350	CA	GLU GLU	43 43	3527	2886	6120	1199 -883 - 152
ANISOU	350	Č	GLU	43	4.701 3454	34.300	54.713	1.000 41.67
ATOM	351	0	GLU	43	3.484	4151 34.124	8229	225 -1743 953
ANISOU		0	GLU	43	3375	4041	7222	1.000 38.53 589 -1417 -578
ATOM ANISOU	352 352	CB	GLU	43	6.278	35.074	53.026	589 -1417 -578 1.000 44.72
ATOM	353	CB CG	GLU GLU	43	5991	4098	6901	28 137 - 2137
ANISOU		CG	GLU	43 43	6.658	36.125	52.003	1.000 53.42
ATOM	354	CD	GLU	43	5931 7.838	6417	7949	-993 1540 -1338
ANISOU		CD	GLU	43	4087	36.976 7601	52.429 7467	1.000 50.41
ATOM	355	OE1	GLU	43	8.024	37.112		-439 2486 -1725 1.000 59.44
ANISOU ATOM		OE1	GLU	43	7237	7592	7757	-1284 1632 -2146
ANISOU	356 356	OE2	GLU	43	8.555	37.476		1.000 71.33
ATOM	357	OE2 N	LEU	43 44	11550	6344	9207	-41316267-4645
ANISOU			LEU	44	5.511 2837	33.373	55.224	1.000 27.80
ATOM	358	CA	LEU	44	4.926	292 <u>4</u> 32.222	4802	-55 $-626$ $-227$
ANISOU		CA	LEU	44	2207	3379	5009	1.000 27.88 241 813 - 382
ATOM ANISOU	359	C	LEU	44	3.886	32.670		241 813 - 382 1.000 34.30
ATOM	360		LEU	44	1930	4771	6333	-537 776 $-2629$
ANISOU	360		LEU LEU	44 44	2.781 2046	32.159	56.924	1.000 33.35
MOTA	361		LEU	44	5.999	5235	5390	-840 705 - 2397
ANISOU	361		LEU	44	2781	31.394 3494	56.587	1.000 24.59
ATOM	362		LEU	44	5.592	30.147	3070 57 343	81 940 - 7 4 1.000 31.76
ANISOU ATOM		CG	LEU	44	2414	5135	4517	-845 792 1217
	363 363	CD1 CD1	LEU	44	4.563	29.328	56.575	1.000 47.71
ATOM	364	CD2	LEU	44 44	5860	7081	5188	-3576 3333 -2541
ANISOU	364	CD2	LEU	44	6.793 6294	29.259 3688	57.653	1.000 51.56
ATOM	365	N	LYS	45	4.212	33.712	9608	1956 2240 1382
	365		LYS	45	2865	6802	6256	1.000 41.91 -1455 381 -3537
ATOM ANISOU	366 366		LYS	45	3.369	34.195		-1455 381 - 3'5 3 7 1.000 44.31
	200	CA	LYS	45	4768	5427		74 837 - 2985
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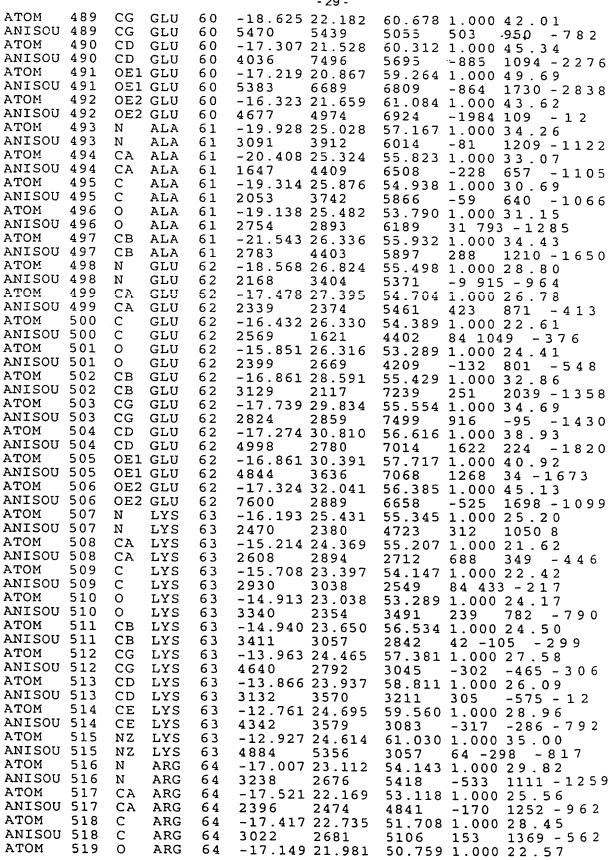
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ATOM	367	С	LYS	45	1.981	34.582	58.278 1.	.000	38.58
ANISOU	367	С	LYS	45	4535	3445			12-2-1 - 2820
MOTA	368	0	LYS	45	0.984	34.238	58.902 1.	.000	39.93
ANISOU	368	0	LYS	45	4857	3594			1634 - 2337
MOTA	369	CB	LYS	45	4.038	35.400	59.447 1.	.000	50.20
ANISOU	369	CB	LYS	45	4944	5561			-447 -3980
ATOM	370	CG	LYS	45	3.082	36.546	59.706 1.	.000	53.07
ANISOU	370	CG	LYS	45	3548	6321	10296 11	148	-2094 -4809
MOTA	371	CD	LYS	45	3.714	37.922	59.622 1.	.000	58.29
ANISOU		CD	LYS	45	4723	5694			-3745 -5024
ATOM	372	CE	LYS	45	3.199	38.793	60.761 1.		
ANISOU		CE	LYS	45	6294	6898			-3430 -5603
MOTA	373	NZ	LYS	45	1.713	38.779	60.852 1.		
ANISOU		ΝZ	LYS	45	6392	9216		718	-1071 -7436
ATOM	374	N	SER	46	1.973	35.341	57.193 1.		
ANISOU		N	SER	46	4074	3478			1068 - 2939
MOTA	375	CA	SER	46	0.743	35.856	56.607 1		
ANISOU		CA	SER	46	3983	3417		1335	
ATOM ANISOU	376	C C	SER SER	46 46	-0.137	34.702	56.137 1. 6602 -3		1656 - 2394
ANISOU	377	0	SER	46	3430 -1.337	3057 34.625	56.449 1		
ANISOU		0	SER	46	3195	2789		.000 587	1093 - 1206
ATOM	378	СВ	SER	46	1.160	36.726	55.419 1		
ANISOU		CB	SER	46	4102	3809		2099	
ATOM	379	ŌĞ	SER	46	0.018	37.017	54.630 1		
ANISOU		ŌĞ	SER	46	5005	3431			53 -1863
ATOM	380	N	ALA	47	0.493	33.808	55.361 1		
ANISOU		N	ALA	47	3246	2173		18	809 -1228
ATOM	381	CA	ALA	47	-0.208	32.623	54.879 1		25.84
ANISOU		CA	ALA	47	3566	2106	4148 7		0 -891
ATOM	382	С	ALA	47	-0.722	31.792	56.058 1		
ANISOU		С	ALA	47	2591	2344		81	280 - 280
ATOM	383	0	ALA	47	-1.888	31.381	56.063 1		
ANISOU		0_	ALA	47	2850	2366	3597 1	29	318 -1119
MOTA	384	CB	ALA	47	0.615	31.791	53.912 1		
ANISOU		СВ	ALA	47	2892	2764	4511 2	70	351 -1134
ATOM	385	N	LYS	48	0.132	31.529	57.041 1	30	-57 <b>-</b> 1085
ANISOU ATOM	386	N	LYS LYS	48 48	3107 -0.186	2076 30.712	4178 1 58.202 1		
ANISOU		CA CA	LYS	48	3545	2979	3291 -	16	30 -1416
MOTA	387	C	LYS	48	-1.337	31.339	59.003 1		
ANISOU		Č	LYS	48	3373	3344		354	
ATOM		ŏ	LYS	48		30.694			
ANISOU		Ŏ	LYS	48	3849	2793			419 -634
ATOM	389	CB	LYS	48	1.035	30.654	59.149 1		
ANISOU		CB	LYS	48	3507	3294		274	
ATOM	390	CG	LYS	48	0.775	29.694	60.313 1		
ANISOU		CG	LYS	48	4412	3214	4897 1	.13	-543 -156
MOTA	391	CD	LYS	48	1.418	30.222	61.570 1		
ANISOU		CD	LYS	48	5828	4616		05	-1278 - 39
ATOM	392	CE	LYS	4.8	1.217	29.320	62.769 1	000	33.67
ANISOU		CE	LYS	48	3973	4020			-205 - 356
ATOM	393	NZ	LYS	48	0.731	30.100	63.946 1		38.33
ANISOU		ΝZ	LYS	48	4516	5230		916	-1039 -1555
ATOM	394	N	ASP	49	-1.253	32.656	59.255 1		23.78 59 -1588
ANISOU ATOM	395	N CA	ASP ASP	49 49	2796 -2.298	3136 33.326	3104 7 60.006 1		
ANISOU		CA		49	2826	2913		 -291	366 -1043
ATOM	396	C	ASP	49	-3.679	33.181	59.366 1		
ANISOU		Ċ	ASP	49	2721	3270		-220	
ATOM	397	Õ	ASP	49	-4.637		60.082		
-				-					•

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ANISO ATOM	ับ 397 398		ASP	49	2863	3177	4257 -368 1004 -1544
ANISO		CB		49 49	2.054		60.167 1.000 30 34
ATOM	399	CG		49	-0.924	3210 35.181	4623 - 559 713 - 2179
ANISO		CG		49	5259	4057	- 1 - 2 - 2 - 1 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0
ATOM ANISO	400		1 ASP	49	-0.556	34.266	4810 -1109 -211 -2007 61.904 1.000 33.36
ATOM	401	מס	1 ASP 2 ASP	49 49	3717	4549	4408 -737 888 -1727
ANISO	J 401	OD.	2 ASP	49	-0.525 7960	36.375 3575	61.087 1.000 48.45
ATOM ANISO	402	N	LEU	50	-3.788	33.402	6875 -927 -2887 -2409 58.059 1.000 24.46
ATOM	403	И СА	LEU LEU	50	3114	2668	3513 374 200 -1202
ANISO		CA	LEU	5 0 5 0	~5.123 2949	33.344 2145	5/.4/1 1.000 22.92
ATOM	404	C	LEU	50	-5.679	31.937	3614 161 397 - 562 57.328 1.000 21.79
ANISOU ATOM	404	C	LEU	50	3345	2197	2737 33 417 -556
ANISOU		Ö	LEU LEU	5 0 5 0	-6.878 3463	31.741	57.475 1.000 24.96
ATOM	406	СВ	LEU	50	-5.254	2502 34.137	3517 -276 766 -1181
ANISOU ATOM		CB	LEU	50	3127	2016	56.194 1.000 22.13 3266 -103 524 -757
ANISOU	407	CG CG	LEU LEU	5 0 5 0	-6.661	34.578	55.807 1.000 28 87
ATOM	408		LEU	50	3549 -7.389	3538 35.082	3881 961 825 208
ANISOU		CD1	LEU	50	4567	8556	57.049 1.000 52.72 6907 940 2929 - 1936
ATOM ANISOU	409	CD2	LEU LEU	50	-6.644	35.642	54.723 1.000 41.07
ATOM	410	N N	VAL	50 51	6971 -4.801	3395 30.956	5240 -1005 -2258 857
ANISOU		N	VAL	51	3345	2052	57.138 1.000 21.78 2877 -160 216 -860
ATOM ANISOU	411 411	CA CA	VAL	51	-5.293	29.580	57.118 1.000 19 40
ATOM	412	C	VAL VAL	51 51	2631 -5.631	2056 29.135	2683 -12 173 -303
ANISOU		C	VAL	51	4453	2656	58.533 1.000 25.25 2485 -753 587 -955
ATOM ANISOU	413 413	0	VAL	51	-6.652	28.454	58.725 1.000 25.07
MOTA	414	СВ	VAL VAL	51 51	4555 -4.377	2176	2795 -484 1185 -827
ANISOU		CB	VAL	51	2729	28.589 1786	56.396 1.000 18.78 2620 -72 171 -313
ATOM ANISOU	415	CG1	VAL	51	-3.152	28.238	2620 -72 171 -313 57.231 1.000 20.42
ATOM	416	CG2	VAL VAL	51 51	3002 -5.147	1841	2918 295 -13 -480
ANISOU	416	CG2	VAL	51	3112	27.306 2337	56.021 1.000 24.10 3708 -511 355 -846
ATOM ANISOU	417	N	ILE	52	-4.836	29.500	3708 -511 355 -846 59.534 1.000 25.23
ATOM	417	N CA	ILE ILE	52 52	4514	2471	2603 388 76 - 974
ANISOU		CA	ILE	52	-5.205 3488	29.114 3010	60.921 1.000 24.38
ATOM	419	C	ILE	52	-6.498	29.771	2765 248 19 - 509 61.355 1.000 24.20
ANISOU ATOM	419	C 0	ILE	52	3026	2482	3687 -354 114 -648
	420	0	ILE	5 2 5 2	-7.328 3735	29.182	62.071 1.000 27.73
ATOM	421	CB	ILE	52	-4.016	2812 29.427	3989 -198 614 -334
ANISOU ATOM	421 422	CB	ILE	52	3321	4347	61.829 1.000 27.59 2815 590 0 -785
ANISOU	422	CG1	ILE ILE	5 2 5 2	-2.853 3278	28.439	61.510 1.000 31.45
ATOM	423	CG2	ILE	52	-4.293	5248 29.312	3425 741 363 -1288
ANISOU ATOM		CG2	ILE	52	3827	6199	63.317 1.000 33.62 2750 881 150 -1454
_	424 424	CD1 CD1	ILE	52	-1.930	28.351	62.710 1.000 36.22
ATOM	425	N	ASP	5 2 5 3	3956 -6.771	5082 30.992	4722 979 -601 - 234
ANISOU	425	N	ASP	53	3479	2878	60.913 1.000 24.56 2974 165 609 -426
ATOM ANISOU	426	CA	ASP	53	-8.051	31.646	2974 165 609 - 426 61.278 1.000 23.50
ATOM	427	CA C	ASP ASP	53 53	3242 -9.201	2942	2745 -5 355 -677
ANISOU	427	Č	ASP	53	3462	30.929 2986	60.594 1.000 26.34 3561 -435 612 -1064
						<del>-</del>	3561 -435 612 -1064

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ATOM	428	0	ASP	5 3	-10.342	30.836	61.051	1.000	29.73
ANISOU	428	0	ASP	5 3	3468	3085		-436	93.71142
MOTA	429	CB	ASP	5 3	-7.964	33.084	60.772	1.000	
ANISOU		CB	ASP	5 3	3800	2322	6730	-92	1806 - 933
ATOM	430	CG	ASP	5 3	-9.308	33.758	60.583	1.000	32.05
ANISOU		CG	ASP	5 3	4652	2412 .		172	-302 -1138
MOTA	431		ASP	5 3	-9.653	34.524	61.486	1.000	43.68
ANISOU	431		ASP	5 3	3661	4686		150	1379 - 3120
MOTA	432		ASP	5 3	-9.950	33.556	59.532	1.000	51.30
ANISOU		OD2	ASP	53	8386	6074			-1738 922
MOTA	433	N	PHE	54	-8.933	30.376	59.413		
ANISOU		N	PHE	5 4	3372	2640			-1176
ATOM	434	CA	PHE	5 4	-9.917	29.557	58.704		
ANISOU		CA	PHE	5 4	3015	3264		-366	263 - 539
ATOM	435	C	PHE	5 4	-10.180		59.456		
ANISOU		C	PHE	54	3264	3174		-365	459 -688
ATOM	436	0	PHE	54	-11.333		59.686		
ANISOU		0	PHE	54	3551	3246	3914	-549	1305 - 1130
ATOM	437	CB	PHE	54	-9.465	29.273	57.263		
ANISOU		CB	PHE	54	3241	2955	2779	-249	218 - 434
ATOM	438	CG	PHE	54	-10.522		56.461		
ANISOU		CG	PHE	54	4712	2945	2838	-694	-636 1 4
ATOM	439		PHE	54	-11.729		56.087		
ANISOU ATOM			PHE	54	3613	4658	3654	-951	-262 - 621
	440		PHE	54	-10.283		56.033		
ANISOU ATOM			PHE PHE	54	5782	3589	2377	-831	293 -844
ANISOU	441			5 <u>4</u> 5 <u>4</u>	-12.653		55.307		
ATOM	441		PHE PHE	54 54	5504 -11.228	5404	5919	-3066	-2057 1178
ANISOU			PHE	54	7997	4412	55.306 2289		
ATOM	443	CZ	PHE	54		27.092	2209 54 007	1 000	155 - 387
ANISOU		CZ	PHE	54	5992	6305	3787		54 - 446
ATOM	444	N	PHE	55	-9.126	27.558	59.870		
ANISOU		N	PHE	55	3787	2768	3276	-85	431 -839
ATOM	445	CA	PHE	55	-9.195	26.310	60.625		
ANISOU		CA	PHE	55	3567	3042	3151		3 - 711
ATOM	446	C	PHE	55	-9.929	26.484			27.69
ANISOU		Č	PHE	55	3357	3961	3205	181	703 - 719
ATOM	447	Ö	PHE	55		25.670			30.08
ANISOU	447	0	PHE	55	4046	4165	3217	142	878 - 127
ATOM	448	CB	PHE	55	-7.759	25.873			25.48
ANISOU	448	CB	PHE	55	3556	3159	2964	117	835 -638
ATOM	449	CG	PHE	55		25.242			26.31
ANISOU	449	CG	PHE	55	3437	3039	3522	-468	1068 - 1156
MOTA	450		PHE	55	-7.611	24.820			27.09
ANISOU	450	CD1	PHE	55	3553	3895	2845	-1018	1404 - 658
MOTA	451		PHE	55	-5.651	25.031	59.935	1.000	31.68
ANISOU			PHE	55	3244	4185	4609	-726	1123 - 2221
ATOM	452		PHE	55	-6.878	24.150	57.621		23.89
ANISOU			PHE	55	3472	2525	3079	-58	551 - 547
ATOM	453	CE2	PHE	55	-4.904	24.433			31.74
ANISOU			PHE	55	3487	4387	4186	226	337 -2304
ATOM	454	CZ	PHE	55	-5.514	24.004			24.23
ANISOU		CZ	PHE	55	3706	2187	3312	414	-22 -416
ATOM	455	N	GLU	56	-9.633	27.581			30.39
ANISOU		N	GLU	56	3961	5033	2553	-308	520 -1110
ATOM	456	CA	GLU	56		27.875			30.18
ANISOU		CA	GLU	56	4160	4504	2805	-734	1221 - 637
ATOM	457	C	GLU	56		28.401			33.50
ANISOU		С	GLU	56	4324	4124	4280	-535	1489 - 892
MOTA	458	0	GLU	56	-12.4/0	28.149	64.708	T.000	) 44.44

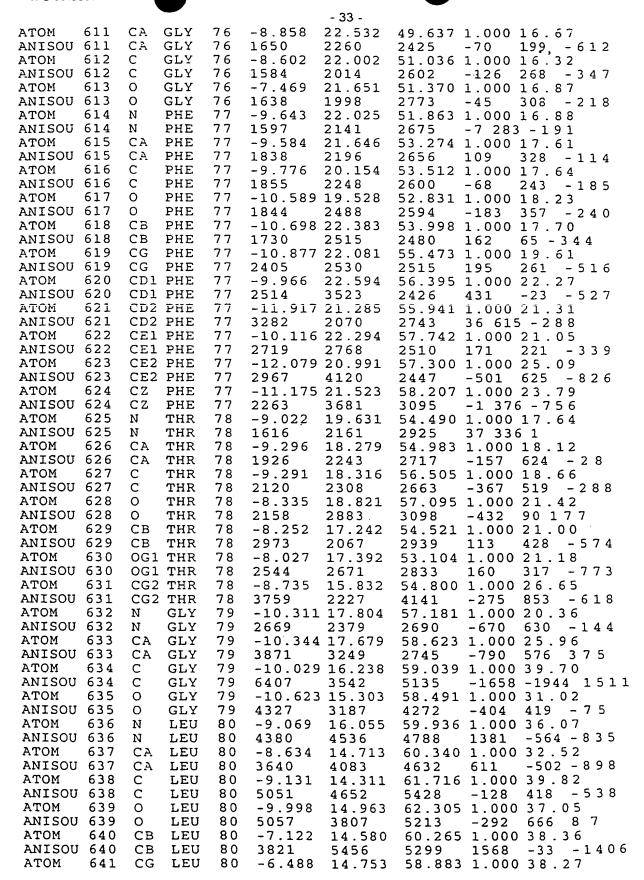
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ANISO		0	GLU		3864	8872	4150	02 1012 101-	
MOTA	459	CB	GLU	56	-9.403	28.978			
ANISO		CB	GLU	56	5037	5109	3475	5 1.000-3-585	
ATOM	460	CG	GLU	56	-8.192	28.508		-221 574 -1821	
ANISO	J 460	CG	GLU	56	4804	7152	05.401	1.000 38.63	
$\mathtt{MOTA}$	461	CD	GLU	56	-7.395	29.699	2721	-337 763 -1692	
ANISOU	J 461	CD	GLU	56	5576	29.699	65.916	5 1.000 45.55	
MOTA	462	OE1	GLU	56	-7.935	7183	4546	-24 -295 -2330	
ANISOU		OE1	GLU	56	7344	30.828	65.888	3 1.000 55.54	
ATOM	463	OE2	GLU	56	-6.246	7247	6512	586 2570 - 3059	
ANISOU		OE2	GLU	56		29.492	66.350	1.000 50.41	
ATOM	464	N	HIS	57	4050	10497	4606	-10661163 - 2063	
ANISOU		N	HIS	57	3273	29.289	62.866	1.000 32.20	
ATOM	465	CA	HIS	57		4700	4261	-549 1540 - 670	
ANISOU		CA	HIS	5 <i>7</i>	-13.TOI	30.078		1.000 33.38	
ATOM	466	C	HIS	5 <i>7</i>	3795	4885	4002	-110 1553 - 1230	
ANISOU		Ċ	HIS		-13.981	29.873		1,000 32 85	
ATOM	467	Ö	HIS	57	3380	4736	4367	278 1506 - 1797	
ANISOU		0		57	-15.012	30.533	61.571	1.000 37 09	
ATOM	468		HIS	57	3362	4733	5998	276 1087 - 2205	
ANISOU		CB	HIS	57	-12.802	31.573	62.976	1.000 37.39	
ATOM	469	CB	HIS	57	4327	4959	4922	-193 1402 - 1970	
ANISOU		CG	HIS	57	-11.981	31.949	64.162	1.000 36.99	
ATOM	470	CG	HIS	57	4111	5046	4896	680 1344 - 2319	
ANISOU	470	MDI	HIS	57	-12.465	31.917	65.453	1.000 38.84	
ATOM	471	MDI	HIS	57	5090	4844	4823	-171 1362 - 1598	
ANISOU	471	CDZ	HIS	57	-10.707	32.387	64.232	1.000 37.91	
ATOM	472	CD2	HIS	57	5259	4197	4947	-891 1544 - 2828	
ANISOU			HIS	57	-11.510	32.305		1.000 40.37	
ATOM			HIS	57	5481	5191	4668	-243 1087 -1361	
ANISOU	473		HIS	57	-10.441	32.592	65.552	1.000 35.63	
ATOM			HIS	57	4420	4376	4743	980 799 -1492	
	474	N	$\mathtt{GLY}$	58	-13.464	29.068		1.000 32.06	
ANISOU ATOM		N	GLY	58	4402	3186	4594	5 1572 -1525	
	475	CA	GLY	58	-14.290	28.731		1.000 35.74	
ANISOU		CA	$\mathtt{GLY}$	58	4508	4402	4669	-1129 1877 - 1893	
ATOM	476	C	GLY	58	-15.449	27.859		1.000 31.52	
ANISOU		С	$\mathtt{GLY}$	58	3317	3688	4969	308 1657 - 593	
ATOM	477	0	GLY	58	-15.245	26.952		1.000 32.66	
ANISOU		0	GLY	58	4561	4176	3674		
ATOM	478	N	SER	59	-16.632	28.152		-204 624 -1012 1.000 31.03	
ANISOU		N	SER	59	3786	3623	4379	519 1142 - 1442	
ATOM	479	CA	SER	59	-17.823	27.359	59 859	1.000 32.03	
ANISOU			SER	59	3305	3925	4939	757 850 -1188	
ATOM	480	С	SER	59	-17.763	26.034	59 117	1.000 37.27	
ANISOU		С	SER	59	3654	4001	6507	0 2065 -1682	
ATOM	481	0	SER	59	-16.987	25.858		1.000 31.23	
ANISOU	_	0	SER	59	3027	3655	5184		
ATOM	482	CB	SER	59	-19.077	28.136		613 1003 - 1174	
ANISOU		CB	SER	59	3930	5925	5266	1.000 39.80 1707 -545 - 2846	
MOTA	483	OG	SER	59	-19.252	28 159		1707 -545 - 2846 1.000 35.38	
ANISOU		OG	SER	59	3505	4800	5137		
ATOM	484	N	GLU	60	-18.589	25 065		355 119 -1624	
ANISOU		N	GLU	60	5438	6083	6078	1.000 46.32	
ATOM	485	CA	GLU	60	-18.573	23 801		-2395 2115 - 2700	
ANISOU			GLU	60	3381	4798	JO. /54	1.000 34.21	
ATOM	486		GLU	60	-19.033	2/30	4818	-960 716 -1238	
ANISOU	486		GLU	60	4659	3711	3/.330	1.000 34.22	
ATOM	487		GLU	60	-18.616	24 422	4632	455 1378 - 847	
ANISOU			GLU	60	3708	3040	26.361	1.000 29.91	
MOTA	488		GLU	60	-19.390	22 742	4615	-679 2037 - 604	
ANISOU	488		GLU	60	5012	5567	27.488	1.000 38.26	
			•			J J G /	3958	-1599 748 -1000	



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ANISOU	519	0	ARG	64	1672	2466	1126		1.40
ATOM	520	СВ	ARG	64		21.809	4436	-71	148 - 395
ANISOU		CB	ARG	64	2669		53.537		· 3 2 . 4 8
ATOM	521	ĊĞ	ARG			4144	5526	-809	1483 -1029
ANISOU				64		20.442	54.189	~1.000	45.55
		CG	ARG	64	4444	4749	8116	-2443	1343 - 153
ATOM	522	CD	ARG	64	-20.557	19.985	54.080	1 000	59.48
ANISOU		CD	ARG	64	5723	6760	10116	-3977	
ATOM	523	NΕ	ARG	64	-20.759	19.485		1 000	-2863 246 <sub>1</sub> 77.63
ANISOU	523	ΝE	ARG	64	10254	9303	9938	4001	//.63
ATOM	524	CZ	ARG	64		20.236		-4031	-4193 2666
ANISOU		CZ	ARG	64	5289		51.696	1.000	60.23
ATOM	525		ARG	64		6952	10644		-4334 501
ANISOU	525		ARG		-21.424	21.528	51.892	1.000	91.64
ATOM	526		ARG	64	18286	5072	11461	-5082	-3134 - 75
				64	-21.286	19.711	50.489	1.000	43.67
ANISOU			ARG	64	3318	4095	9178	-183	-1521 2085
ATOM	527	N	ALA	65	-17.624	24.041	51.515	1 000	26 71
ANISOU		N	ALA	65	1907	2770	5472	189	936 - 556
$\mathtt{ATOM}$	528	CA	ALA	65	-17.522	24 661	50.199	1 000	24 01
ANISOU		CA	ALA	65	1798	2379	5288	1.000	
ATOM	529	С	ALA	65	-16.109	24 575		280	417 - 754
ANISOU	529	C	ALA	65	1808	24.5/5	49.595	1.000	
ATOM	530	ŏ	ALA	65		2408	4071	597	155 -626
ANISOU		Ö	ALA		-15.935		48.381	1.000	24.13
ATOM	531			65	2127	3076	3964	224	-220 -485
		CB	ALA	65	-18.023	26.096	50.221	1.000	31.78
ANISOU		CB	ALA	65	3096	2984	5993	1337	1401 - 453
ATOM	532	N	VAL	66	-15.098	24.306	50.426	1.000	19 29
ANISOU		N	VAL	66	1836	1880	3614	466	360 - 541
ATOM	533	CA	VAL	66	-13.723	24.167	49.953		18.17
ANISOU	533	CA	VAL	66	1636	1653	3616	204	
ATOM	534	С	VAL	66	-13.166	22 767		204	79 - 487
ANISOU	534	С	VAL	66	1516		50.248	1.000	15.18
MOTA	535	ō	VAL	66		1638	2613	120	126 -571
ANISOU		ŏ	VAL		-11.939	22.623	50.353	1.000	17.63
ATOM	536	СВ		66	1567	2071	3060	217	-106 - 317
ANISOU			VAL	66	-12.784		50.437	1.000	18.91
		CB	VAL	66	2175	1576	3433	183	-135 - 598
ATOM	537		VAL	66	-13.139	26.627	49.805		20.60
ANISOU			VAL	66	2067	1751	4010	219	593 - 83
ATOM	538		VAL	66	-12.736	25.373	51.945		21.61
ANISOU	538	CG2	VAL	66	2689	2066	3455	102	22 - 603
ATOM	539	N	THR	67		21.792	50 242	1 000	
ANISOU	539	N	THR	67	1761	1614	3577		18.30
ATOM	540	CA	THR	67	-13.673	1014		-20	-6 -514
ANISOU		CA	THR	67	1927		50.563		
ATOM	541	C	THR			1656	2946	-32	50 - 556
ANISOU		C		67	-13.979		49.332	1.000	16.52
ATOM			THR	67	1763	1742	2773	21 27	-467
	542	0	THR	67	-15.107	19.613	48.811	1.000	18.13
ANISOU		0		67	1750	2211	2929	73 -86	5 - 3 8 3
ATOM	543	CB	$\mathtt{THR}$	67	-14.373		51.782	1 000	10 51
NOSINA		CB	THR	67	2202	2014	2827	192	224 - 492
MOTA	544	OG1	THR	67	-14.060	20 554		1 2 2	224 - 492
ANISOU	544	OG1		67	2481	2251	52.961		
ATOM	545	CG2		67	-13.912	10 264	2920	-108	155 - 468
ANISOU		CG2		67	2393		52.017	1.000	20.04
ATOM	546	N				2016	3203	29 -86	5 - 2 3 5
ANISOU	546		SER	68	-13.030		48.821	1.000	16.71
ATOM		N	SER	68	1612	1720	3018	-135	154 - 498
	547	CA	SER	68	-13.281	17.947	47.688	1.000	16.33
ANISOU		CA	SER	68	1508	1631	3065	-184	365 - 561
MOTA	548	С	SER	68	-14.223	16.795	48.057		14.85
ANISOU	548	С	SER	68	1194	1775	2672	-81	
ATOM	549	0	SER	68	-14.303	16 431		- O T	197 - 448
ANISOU	549	0	SER	68	1783	1775	49.233	T.000	
-	-	-			- 703	1113	2659	-145	192 - 481

АТОМ	550	СВ	SER	68 -	-11.958	17.303	47.257	1.000 17.84
ANISOU							3182 -	-87 647313
MOTA	551	OG	SER		-10.998			1.000 17.21 -75 364 - 49
ANISOU			SER		1659 -14.929	1987		-75 364 - 49 1.000 15.89
MOTA	552		PRO			16.284		-201 -103 -280
ANISOU ATOM	553	N CA	PRO PRO	69	-15.877			1.000 16.42
ANISOU		CA	PRO			1903	2908	-251 -148 -218
ATOM	554	C	PRO		-15.168			1.000 17.22
ANISOU		C	PRO			1578	3331	-199 266 -424 1.000 18.35
MOTA	555	0	PRO		-15.794 1815	1760	3399	-365 232 -376
ANISOU ATOM	555 556	O CB	PRO PRO		-16.712			1.000 16.75
ANISOU		CB	PRO		1354	2279	2733	-360 155 -729 .
MOTA	557	ĊĠ	PRO	69	-15.799			1.000 16.72
ANISOU		CG	PRO		1553	1971		-359 38 -452
MOTA	558	CD	PRO		-15.059	16.797		1.000 17.10 -344 -119 -313
ANISOU		CD N	PRO VAL	69 -70	1918 -13.884			1.000 18.07
ATOM ANISOU	559 559	N	VAL	70	1716	1764	3384	-89 292 -215
ATOM	560	CA	VAL	70	-13.100	12.594		1.000 17.34
ANISOU	560	CA	VAL	70	1763	1851	2974	-20 260 -196
MOTA	561	C	VAL	70	-11.995			1.000 17.59 -180 159 -142
ANISOU		C	VAL VAL	70 70	2207 -11.431	1686	2788 48 389	1.000 18.59
ATOM ANISOU	562 562	0	VAL	70	1794	1688	3581	-4 9 152
ANISOU	563	СВ	VAL	70	-12.429		46.724	1.000 18.10
ANISOU		СВ	VAL	70	1922	1756	3199	-353 560 -446
ATOM	564		VAL	70	-13.441			1.000 20.54 -369 76 -663
ANISOU			VAL	70	1927 -11.760	2611	3268 45 642	-369 76 -663 1.000 17.65
ATOM ANISOU	565		VAL	70 70	2379	1806	2520	145 9 1 0
ANISOU	566	N N	PRO	71	-11.697		49.815	1.000 16.21
ANISOU		N	PRO	71	1653	1810	2695	-34 464 -156
MOTA	567	CA	PRO	71		13.091		1.000 17.32 -121 184 - 12
ANISOU		CA	PRO	71	1795 -9.356	1931 12.804	2854	-121 184 - 12 1.000 17.67
ATOM ANISOU	568 568	C	PRO PRO	71 71	1865	1927	2921	46 -57 1 5 6
ANISOC	569	Õ	PRO	71	-8.585	12.223	51.350	1.000 20.57
ANISO		Ö	PRO	71	2218	2247	3350	424 28 4 7 4
MOTA	570	CB	PRO	71		12.458		1.000 19.76 -347 479 -304
ANISO		CB	PRO	71	2976	1862 11.056	2668	-347 479 -304 1.000 19.08
ATOM	571	CG CG	PRO PRO	71 71	2838	1805	2608	-267 259 -234
ANISOU ATOM	572	CD	PRO	71	-12.32	3 11.220	50.286	1.000 17.97
ANISO		CD	PRO	71	2314	1974	2538	-390 451 -167
MOTA	573	N	THR	72	-8.894	13.338		5 1.000 17.15
ANISO		N	THR	72	1677	2231	2610	-215 -17 -165 5 1.000 16.83
ATOM	574	CA CA		72 72	-7.573 1721	13.012 1863	2810	-60 -134 - 472
ANISO ATOM	575 575	C	THR		-6.490	14.000		3 1.000 15.20
ANISO			THR		1791	1623 .	2362	-304 163 -73
ATOM	576	0	THR		-5.320			4 1.000 17.49 -61 -31 -225
ANISO			THR		1776	1961	2908	
ATOM	577				-7.533 1552	12.971 1848	. 47.39! 2748	-146 -86 -261
ANISO ATOM	578		THR THR		-8.091			5 1.000 17.81
ANISC			THE		1856	1880	3031	-34 115 -191
ATOM	579	CG	2 THE	72	-8.338			5 1.000 17.49
ANISC			2 THE			2087	2605	-550 181 -329 7 1.000 17.78
MOTA	580	) И	MET	73	-6.877	15.09	5 47.78	/ 1.000 17.78



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ANISO		CG		80	3714	5900	4926	72= 200 2=00
ATOM	642		1 LEU	80	-5.007	14.359	58.948	725 -288 -2589 1.000 45.41
ANISO			1 LEU	80	2579	8505	6170	- · - <del>-</del>
ATOM	643		2 LEU	80	-7.170	13.856		-1092 -76 3 7 1.000 40.75
ANISOU ATOM			2 LEU	80	4296	5601	5587	872 -1965 -1793
ANISOU	644	N	SER	98	-6.459	17.442		1.000 36.72
ATOM	645	N CA	SER	98	3404	6429	4118	-2114 -698 1942
ANISOU		CA	SER SER	98	-5.629	17.877	62.824	1.000 39.59
ATOM	646	C	SER	98 98	6031	5376	3635	-449 383 2177
ANISOU	J 646	Č	SER	98	-6.402 3806	18.372	61.610	1.000 29.89
ATOM	647	Ō	SER	98	-7.474	3509 17.856	4040	141 640 1204
ANISOU	647	0	SER	98	4936	4300	5303	1.000 38.27
ATOM	648	СВ	SER	98	-4.694	16.739	62 350	-1107 395 885 1.000 44.06
ANISOU		CB	SER	98	3175	7425	6141	633 -753 2704
ATOM ANISOU	649	OG	SER	98	-3.672	17.368	61.583	1.000 46.84
ANISOU	650	OG	SER	98	3497	6502	7797	95 -408 2418
ANISOU		N N	MET	99	-5.829	19.317	60.869	1.000 28.56
ATOM	651	CA	MET MET	99 99	5029	3458	2365	-1080 -550 5 4 6
ANISOU		CA	MET	99	-6.426 2284	19.941	59.700	1.000 21.44
ATOM	652	Č	MET	99	-5.376	3549 20.229	2315	-182 157 132
ANISOU	652	С	MET	99	2306	2592	58.624	1.000 19.16
ATOM	653	0	MET	99	-4.232	20.575	2382	-433 60 1 3 7
ANISOU		0	MET	99	2489	3920	2460	1.000 23.34 -773 225 -410
ATOM	654	CB	MET	99	-7.164	21.209		-773 225 -410 1.000 25.20
ANISOU ATOM	654 655	CB	MET	99	3172	3375	3028	-572 661 -547
ANISOU		CG CG	MET MET	99	-8.481	20.965	60.872	1.000 25.85
ATOM	656	SD	MET	99 99	3172 -9.251	3862	2787	-275 739 - 782
ANISOU		SD	MET	99	4405	22.517 3750	61.389	1.000 32.21
ATOM	657	CE	MET	99	-8.884	22.461	4083	-133 1580 - 568
ANISOU		CE	MET	99	14782	11538	2603	1.000 76.12
ATOM	658	N	CYS	100	-5.778	20.094	57 361	-3321 3478 -3241 1.000 18.85
ANISOU		N	CYS		2434	2443	2285	-160 93 1 9 4
ATOM ANISOU	659	CA	CYS		-4.868	20.333		1.000 18.55
MOTA	660	CA C	CYS CYS		2251	2380	2418	92 127 2 3 6
ANISOU	660	C	CYS	100	-5.496 1826	21.312	55.228	1.000 16.26
ATOM	661	Õ	CYS		-6.728	2031	2321	110 329 2
ANISOU		Ō	CYS	100	1741	21.308 2395	55.071	1.000 17.69
ATOM	662	CB	CYS	100	-4.604	18.982	2586	-69 154 -104
ANISOU		CB	CYS	100	2822	2081		1.000 18.46 98 118 5 1 1
ATOM	663	SG	CYS		-3.243	18.974		1.000 22.76
ANISOU ATOM	664	SG	CYS		2622	2968	3058	307 391 1 0
ANISOU		N N	TYR	101	-4.697	22.069	54.498	1.000 17.49
ATOM	665	CA	TYR TYR		1839	2473	2332	46 291 2 2 4
ANISOU		CA	TYR		-5.117 1946	22.874		1.000 15.38
ATOM	666	C	TYR		-4.102	1939 22.594	1960	-50 90 - 262
ANISOU		С	TYR	101	1676	1543	1967	1.000 13.65
ATOM	667	0	TYR		-2.896	22.629		-2 -123 -151 1.000 15.95
ANISOU		0	TYR	101	1611	2231		-43 -232 - 212
ATOM ANISOU	668	CB	TYR		-5.122	24.382	53.739	1.000 19.02
ATOM	668 669	CB	TYR		2816	2082	2328	234 48 - 519
ANISOU	669	CG CG	TYR TYR		-5.617	25.109	52.498	1.000 17.85
ATOM	670		TYR		2084 -6.964	1895	2804	18 -26 -231
ANISOU	670		TYR	101	2042	25.134 1596	52.171	1.000 18.25
ATOM	671	CD2	TYR		-4.730	25.778	3298	29 28 - 496
ANISOU	671	CD2	TYR	101	2037	1611		1.000 17.77 -46 -125 - 127
							-	127 121

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MOTA	672	CE1	TYR	101	-7.406	25.796	51 036	1.000 19.63
ANISOU	672		TYR		1977	1776	3704	88 -241 - 221
ATOM	673		TYR		-5.147	26.386		1.000 20.46
ANISOU	673		TYR		2060	2608	3108	239 40 182
ATOM	674	CZ	TYR		-6.504	26.392		1.000 20.29
ANISOU	674	CZ	TYR		2187	2397	3127	-73 -353 - 260
ATOM	675							
		OH	TYR		-6.932	26.995	49.000	
ANISOU	675	ОН	TYR		2790	2555	3523	-3 -641 5 2
ATOM	676	N	SER		-4.648	22.210		1.000 14.60
ANISOU	676	N	SER		1618	1890	2041	-61 -109 -477
ATOM	677	CA	SER		-3.797	21.792		1.000 14.52
ANISOU		CA	SER		1684	1802	2030	-108 62 - 276
MOTA	678	С	SER		-4.011	22.670	48.747	1.000 14.99
ANISOU	678	С	SER	102	1545	1790	2361	-296 -41 2 1
MOTA	679	0	SER	102	-5.167	23.105	48.477	1.000 16.73
ANISOU	679	0	SER	102	1589	2342	2425	2 128 - 3
ATOM	680	CB	SER	102	-4.163	20.340	49.593	1.000 13.82
ANISOU	680	CB	SER	102	1692	1548	2013	174 9 -138
ATOM	681	OG	SER		-3.996	19.476		1.000 16.06
ANISOU		ŌĠ	SER		1886	2066	2153	97 -121 6 3
ATOM	682	N	MET		-2.978	22.775	47.920	
ANISOU		N	MET		1568	1724	2206	51 -59 1 5 2
ATOM	683	CA	MET		-3.102	23.552		1.000 16.58
ANISOU	683	CA	MET		2194	1933	2173	
ATOM	684	C	MET		-2.150	23.013		
ANISOU		c			1598			1.000 14.41
			MET			1793	2083	-202 -210 6 3
ATOM	685	0	MET		-1.157	22.347	45.920	
ANISOU	685	0	MET		1527	2384	2259	-61 -23 468
MOTA	686	CB	MET		-2.716	25.004		1.000 28.78
ANISOU		CB	MET		6537	1318	3081	859 -207 3 6 6
ATOM	687	CG	$\mathtt{MET}$		-3.258	25.986		1.000 22.60
ANISOU	687	CG	$\mathtt{MET}$		2531	2157	3900	-161 -57 -291
MOTA	688	SD	MET		-2.338	27.505		1.000 20.60
ANISOU	688	SD	$\mathtt{MET}$	103	2499	1927	3400	-4 -164 -226
$\mathtt{ATOM}$	689	CE	MET	103	-2.587	27.945	45.804	1.000 21.63
ANISOU	689	CE	MET	103	2319	2601	3300	308 209 - 236
MOTA	690	N	$\mathtt{GLY}$	104	-2.439	23.430	44.378	1.000 15.44
ANISOU	690	N	${ t GLY}$	104	1468	2228	2169	-68 -120 1 6 4
MOTA	691	CA	GLY	104	-1.511	23.199		1.000 16.13
ANISOU		CA	GLY		1688	2202	2241	42 65 4 6 9
MOTA	692	C	GLY		-1.583	24.355		1.000 15.76
ANISOU	692	Č	GLY		1706	1997	2286	-32 -194 3 8 8
ATOM	693	Õ	GLY		-1.987	25.478		1.000 19.06
ANISOU		ŏ	GLY		1953	2032	3256	-71 144 3 3 3
ATOM	694	N	THR		-1.151	24.092		1.000 16.73
ANISOU		N	THR	105	1685	2385	2287	-375 -55 515
ATOM	695	CA	THR		-1.115	25.205		
								1.000 17.06
ANISOU		CA	THR	105	1725	2390	2369	-231 -148 5 7 7
ATOM	696	C	THR		-2.513	25.631		1.000 19.55
ANISOU		C	THR	105	1768	1817	3842	-160 -346 5 2 5
ATOM	697	0	THR		-2.680	26.703		1.000 22.41
ANISOU		0	THR	105		2116	4136	-119 -520 8 4 2
ATOM	698	CB	THR	105	-0.301	24.857		1.000 17.57
ANISOU		СВ	THR	105	1759	2877	2038	-394 -343 377
ATOM	699		THR	105	-0.865	23.675		1.000 18.66
ANISOU	699		THR	105	2035	2449	2607	-140 -458 4 1 6
MOTA	700	CG2	THR	105	1.155	24.590		1.000 18.95
ANISOU	700		THR	105	1748	2853	2601	-105 -248 2 9 6
ATOM	701	N	ALA		-3.507	24.751		1.000 16.52
ANISOU		N	ALA		1596	2293	2389	-180 -1 2 9 8
ATOM	702	CA	ALA		-4.846	25.035		3 1.000 16.59
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ANISOU 702	CA ALA	106 1600	- 36 -	
ATOM 703			1952	2660 -214 -209 2 4 3
ANISOU 703				39.923 1.000 4.7, 52
ATOM 704			1821	3186 26 -66 5 5 5
ANISOU 704		106 -5.479	23.323	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ATOM 705			2087	
ANISOU 705		106 2331	24.838	
ATOM 706	N ASP		2764	2620 -197 -403 4 4 0
ANISOU 706	N ASP	107 1576	24.329 2208	1 1 2 3 3 3 2 3 3 0 0
ATOM 707	CA ASP		23.535	3057 -77 -120 4 9
ANISOU 707	CA ASP		2191	
ATOM 708	C ASP	107 -8.173	23.753	
ANISOU 708		107 1825	2044	2-1-1-2 2:000 27.74
ATOM 709		107 -8.458	22.854	2869 447 -269 3 6 2 42.650 1.000 18.95
ANISOU 709	O ASP	107 1994	2230	2974 167 -133 4 0 2
ATOM 710 ANISOU 710	CB ASP	107 -8.089	22.044	39.990 1.000 19.62
ATOM 711	CB ASP	107 2213	2300	2942 -394 -727 1 7 3
ANISOU 711	CG ASP	107 -8.370	21.842	38.508 1.000 20 81
ATOM 712	CG ASP OD1 ASP	107 1952	3093	2862 -138 -532 - 14
ANISOU 712	OD1 ASP	107 -9.369 107 2524	22:369	37.976 1.000 25 84
ATOM 713	OD2 ASP	107 2524	3967	3327 222 -1149 - 240
ANISOU 713	OD2 ASP	107 3314	21.168	37.844 1.000 25.86
ATOM 714	N ASN	107 3314	2989	3523 391 -91 - 00
ANISOU 714	N ASN	108 2049	24.962 2075	42.298 1.000 18.18
ATOM 715	CA ASN	108 -7.831	25.263	2786 509 189 153
ANISOU 715	CA ASN	108 1804	1977	43.740 1.000 17.10 2715 266 291 3.27
ATOM 716	C ASN	108 -9.158	25.716	2715
ANISOU 716 ATOM 717	C ASN	108 1705	2061	2734 367 44 1 4 9
ATOM 717 ANISOU 717	O ASN O ASN	108 -10.103	26.086	43.604 1.000 20.72
ATOM 718	O ASN CB ASN	108 2066	2377	3430 759 -248 245
ANISOU 718	CB ASN	108 -6.799 108 1770	26.379	43.969 1.000 19.90
ATOM 719	CG ASN	108 1770	2308	3483 186 298 -171
ANISOU 719	CG ASN	108 1709	25.862 2212	43.717 1.000 17.24
ATOM 720	OD1 ASN	108 -4.986	24.850	2628 200 68 1 8 4
ANISOU 720	OD1 ASN	108 2003	1984	44.277 1.000 17.42 2631 109 11 - 62
ATOM 721	ND2 ASN	108 -4.644	26.487	
ANISOU 721	ND2 ASN	108 2083	2326	42.834 1.000 18.41 2587 -82 300 - 18
ATOM 722	N LEU	109 -9.308	25.509	2587 -82 300 - 18 45.607 1.000 18.09
ANISOU 722 ATOM 723	N LEU	109 1795	2294	2786 240 244 7 0
ATOM 723 ANISOU 723	CA LEU	109 -10.532	25.803	46.369 1.000 19.11
ATOM 724	CA LEU C LEU	T 0 7 T 1 0 3	2200	3296 14 476 - 598
ANISOU 724	· C LEU	109 -10.169	26.790	47.457 1.000 17.40
ATOM 725	O LEU	109 1682 109 -9.443	1937	2990 251 129 - 207
ANISOU 725	O LEU	109 2443	26.423	48.395 1.000 21.18
ATOM 726	CB LEU	109 -11.100	1922	3684 174 -520 2
ANISOU 726	CB LEU	109 1888	2142	46.940 1.000 17.10
ATOM 727	CG LEU	109 -11.520	23 425	2469 199 426 -630
ANISOU 727	CG LEU	109 2515	1943	45.944 1.000 18.07 2409 190 -198 - 363
ATOM 728	CD1 LEU	109 -11.895	22.124	2409 190 -198 - 363 46.654 1.000 20.06
ANISOU 728 ATOM 729	CD1 LEU	109 2842	2406	2375 -331 -175 - 200
ATOM 729 ANISOU 729	CD2 LEU	109 -12.630	23.908	45.035 1.000 25.24
ATOM 730	CD2 LEU N PHE	109 3481	2892	3217 306 -992 -111
ANISOU 730	N PHE N PHE	110 -10.609		47.313 1.000 17.25
ATOM 731	CA PHE	110 1584 110 -10.235	1926	3045 272 184 - 132
ANISOU 731	CA PHE	110 -10.235	1816	48.277 1.000 18.20
ATOM 732	C PHE	110 -11.409	29 567	3346 169 221 -160
ANISOU 732	C PHE	110 2077	1609	49.106 1.000 19 93 3886 71 650 - 335
				3886 71 650 - 335

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ATOM	733	0	PHE	110	-12.433	29.948	48.494	1.000	24 64
ANISOU	733	0	PHE		2051	2461		612	
ATOM	734	СB	PHE		-9.607	30.243	47.520	1 000	19 92
ANISOU	734	CB	PHE	110	2367	1876		224	619 - 93
ATOM	735	CG	PHE		-8.380	29.986	46.688		
	735	CG	PHE		2009	2209	3179		
	736	CD1						-321	327 - 791
ATOM		_			-7.177	29.680	47.287		
ANISOU		CD1			2071	2080	3674	-274	236 - 331
ATOM	737	CD2			-8.437	30.035	45.299		
	737	CD2			2557	1914	3200	112	543 -289
ATOM	738	CE1			-6.034	29.454			21.06
	738	CE1			2020	2309	3673	-386	165 -622
MOTA	739	CE2			-7.277	29.811	44.547	1.000	
ANISOU	739	CE2	PHE	110	2495	2138	3257	197	504 - 398
MOTA	740	CZ	PHE	110	-6.081	29.518	45.175	1.000	22.42
ANISOU	740	CZ	PHE	110	2747	2092	3678	531	339 - 357
MOTA	741	N	PRO	111	-11.238	29.718	50.416	1.000	
ANISOU	741	N	PRO		2250	2153	3996	-72	871 -620
MOTA	742	CA	PRO		-12.287				28.23
ANISOU	742	CA	PRO		3895	2210	4621	698	1514 - 671
ATOM	743	C	PRO		-12.333		50.784		
	743	č	PRO		4528	2026	5061	410	410 -1041
ATOM	744	Ö	PRO		-11.390		50.115		
ANISOU	744	Ö	PRO		4040	2236	5774	-179	
ATOM	745	CB	PRO						-597 - 1 2
ANISOU					-11.799		52.627		
		CB	PRO		5609	2702	4303	671	1671 - 790
ATOM	746	CG	PRO		-10.646		52.647		
ANISOU	746	CG	PRO		2742	3316	3835	-931	1324 - 192
ATOM	747	CD	PRO		-10.161		51.230		
ANISOU	747	CD	PRO		2587	2307	3522	-471	541 -623
MOTA	748	N	SER		-13.337		51.150		
ANISOU	748	N	SER		7176	2716	6115	2074	1731 - 526
MOTA	749	CA	SER		-13.368		50.672		
ANISOU	749	CA	SER		6799	2255	7684	1107	-485 -826
$\mathtt{ATOM}$	750	С	SER		-13.262	34.157	49.149	1.000	68.28
UOZINA	750	С	SER		13632	4498.	7812	-1855	-2077 1301
MOTA	751	0	SER	112	-12.347	34.825	48.646	1.000	95.18
ANISOU	751	0	SER	112	15991	11425	8747	-4337	-70 1985
MOTA	752	CВ	SER	112	-12.493	35.069	51.349	1.000	39.31
ANISOU	752	СВ	SER		2247	4535	8153	580	1662 - 1437
ATOM	753	OG	SER		-11.474		52.213	1.000	
ANISOU	753	ŌĞ	SER		7213	2453	4579	806	747 -1152
ATOM	754	N	ASP		-9.515				36.40
ANISOU		N	ASP		3476	2118	8237	1254	
ATOM	755	CA	ASP		-8.205	37.586			30.79
ANISOU		CA	ASP		3503	2856	5340	1229	1240 9 9 6
ATOM	756	C	ASP		-7.242	36.402			26.16
ANISOU		Ċ	ASP		2581	2404	4955	601	1114 8 0 4
ATOM	757	0			-6.031				
			ASP			36.458			25.45
ANISOU		0	ASP		2302	2503	4866	-43	602 131
ATOM	758	CB	ASP		-8.595	37.874		1.000	43.68
ANISOU		CB	ASP		7509	2783	6304	1157	2727 - 210
ATOM	759	CG	ASP		-7.391	38.386			46.96
ANISOU		CG	ASP		9259	3225	5359	2517	519 107
ATOM	760		ASP		-6.487	38.959	52.189		83.49
ANISOU			ASP		13724	9866	8132	-6354	
MOTA	761		ASP		-7.370	38.262	54.071		0113.59
ANISOU		OD2	ASP		27880	10550	4730		1 -159 -2575
ATOM	762	N	PHE	115	-7.831	35.323			22.32
ANISOU	762	N	PHE	115		2062	3799	204	954 -114
ATOM	763	CA	PHE	115	-7.115	34.026	51.183		22.69

ANISOU 763 CA PHE 115 2655 1009 3947 118 1093 -187 ANISOU 764 C PHE 115 -6.502 33.754 49.816 1.000 20.51 ANISOU 765 O PHE 115 -5.328 33.3754 3702 305 559 -255 ANISOU 765 O PHE 115 -5.328 33.754 3702 305 559 -255 ANISOU 766 CB PHE 115 2153 2011 3627 323 488 -158 ANISOU 766 CB PHE 115 2153 2011 3627 323 488 -158 ANISOU 767 CG PHE 115 -7.496 31.590 51.998 1.000 20.76 ANISOU 767 CG PHE 115 -6.9915 30.74 36374 -3.7563 -473 ANISOU 768 CD1 PHE 115 -6.9915 30.74 36374 -3.7563 -473 ANISOU 768 CD1 PHE 115 -6.9915 30.74 36374 -3.7563 -473 ANISOU 769 CD2 PHE 115 -6.9915 30.74 363374 -3.7563 -473 ANISOU 769 CD2 PHE 115 -6.9915 30.74 36374 -3.7563 -473 ANISOU 769 CD2 PHE 115 -6.9915 30.74 36374 -3.7563 -473 ANISOU 770 CE1 PHE 115 -6.9915 30.74 36374 -3.7563 -473 ANISOU 770 CE1 PHE 115 -6.9915 30.74 36374 -3.7563 -473 ANISOU 770 CE1 PHE 115 -6.9315 29.913 ANISOU 770 CE1 PHE 115 -6.9312 29.913 ANISOU 770 CE2 PHE 115 -6.9312 29.913 ANISOU 771 CE2 PHE 115 -6.9312 29.913 ANISOU 773 N GLU 116 -2396 12.92 ANISOU 775 C GLU 116 -6.7503 33.764 342 44 44 4.000 20.90 ANISOU 775 C GLU 116 -6.7505 ANISOU 777 CB GLU 116 -6.7503 33.404 43 43.7572 ANISOU 777 CB GLU 116 -6.7503 33.3404 44 3.7572 ANISOU 778 CG GLU 116 -6.7503 33.3404 47.444 1.000 20.90 ANISOU 778 CG GLU 116 -6.7505 31.3504 33.3504 43.3507 -10.000 21.16 ANISOU 779 CD GLU 116 2209 21.47 ANISOU 778 CG GLU 116 -7.851 33.350 42.262 47.444 1.000 20.90 ANISOU 778 CG GLU 116 -7.851 33.3504 43.3507 -10.000 21.87 ANISOU 778 CG GLU 116 -7.851 33.3504 -3.7504 779 CD GLU 116 -2405 20.7504 40.7504 10.000 20.32 ANISOU 778 CG GLU 116 -7.851 33.3504 44.262 47.444 1.000 20.90 ANISOU 778 CG GLU 116 -7.851 33.3504 47.350 -0.000 21.87 ANISOU 779 CD GLU 116 2209 41.64 48.94 47.31 3.99 ANISOU 778 CG GLU 116 -7.851 33.3504 47.350 -0.000 21.87 ANISOU 779 CD GLU 116 2405 20.900 33.3504 47.350 -0.000 21.87 ANISOU 779 CD GLU 116 2405 20.900 33.3504 47.350 -0.000 21.87 ANISOU 778 CG GLU 116 -7.851 33.3504 47.350 -0.000 20.18 ANISOU 788 CAR MIT 7.3045 47.304 47.304 77.304 77.304 77.304 77.304 77.304 77.304				- 38 -	
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ANISOU 776 CG PHE 115 27.496 31.590 51.998 1.000 20.23 ANISOU 767 CG PHE 115 26.915 30.756 ANISOU 768 CDI PHE 115 26.915 30.756 ANISOU 769 CD2 PHE 115 26.291 1786 3372 -195 112 -756 ANISOU 770 CEI PHE 115 26.351 29.538 51.325 1.000 21.09 ANISOU 770 CEI PHE 115 26.351 29.538 51.325 1.000 21.09 ANISOU 771 CE2 PHE 115 26.351 29.538 51.325 1.000 21.09 ANISOU 771 CE2 PHE 115 -6.351 29.538 51.325 1.000 21.09 ANISOU 772 CZ PHE 115 -6.351 29.518 51.325 1.000 21.09 ANISOU 773 N GLU 116 2.396 1.899 ANISOU 774 CA GLU 116 -7.301 33.768 48.757 1.000 21.64 ANISOU 775 C GLU 116 2.355 1.895 3.390 318 261 -13 ANISOU 775 C GLU 116 27.301 33.464 44 43 -57 2 ANISOU 775 C GLU 116 27.301 33.464 44 43 -57 2 ANISOU 775 C GLU 116 27.301 33.464 44 43 -57 2 ANISOU 775 C GLU 116 27.301 33.464 44 43 -57 2 ANISOU 775 C GLU 116 27.301 33.468 48.757 1.000 21.64 ANISOU 776 C GLU 116 27.301 33.464 44 43 -57 2 ANISOU 775 C GLU 116 27.301 33.464 44 43 -57 2 ANISOU 775 C GLU 116 27.301 33.468 48.757 1.000 21.64 ANISOU 776 C GLU 116 27.301 33.468 48.757 1.000 21.64 ANISOU 776 C GLU 116 27.301 33.468 48.757 1.000 21.64 ANISOU 776 C GLU 116 27.301 33.468 48.757 1.000 21.64 ANISOU 776 C GLU 116 2425 2638 41.39 41.40 48 ANISOU 777 C G GLU 116 2425 2638 41.39 46.600 20.32 ANISOU 777 C G GLU 116 2425 2638 41.39 46.600 20.32 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 778 C G GLU 116 2425 2638 41.39 46.70 -23.7 519 ANISOU 780 C C ARG 11.7 2.30 53.50 579 470 -23.7 519 97 ANISOU 780 C C ARG 11.7 2.30 53.50 579 470 -23.7 519 97 ANISOU 780 C C ARG 11.7 2.3			0.000		51.638 1.000 20.76
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ANISOU 768 CD1 PHE 115 2672 1786 ANISOU 769 CD2 PHE 115 2572 1786 ANISOU 769 CD2 PHE 115 2572 1786 ANISOU 776 CD2 PHE 115 2672 1786 ANISOU 7770 CE1 PHE 115 2602 1783 377 ANISOU 770 CE1 PHE 115 2602 1783 377 ANISOU 770 CE1 PHE 115 2602 1783 3782 -195 112 -7756 ANISOU 771 CE2 PHE 115 2602 1728 3784 -295 471 -538 ANISOU 771 CE2 PHE 115 6.351 29.518 ANISOU 771 CE2 PHE 115 6.351 29.518 ANISOU 772 CZ PHE 115 6.352 29.518 ANISOU 773 N GLU 116 -7.351 1889 4222 50 1519 22 1 ANISOU 774 CA GLU 116 2396 1835 3990 338 261 -13 ANISOU 775 C GLU 116 2396 1835 3990 338 261 -13 ANISOU 775 C GLU 116 2555 34.262 47.054 1.000 20.990 ATOM 775 C GLU 116 2555 34.262 47.054 1.000 20.32 ATOM 776 O GLU 116 2454 33.667 444 1.000 20.990 ATOM 777 CB GLU 116 2454 33.667 444 1.000 20.18 ATOM 778 CG GLU 116 2425 2638 4139 -108 44 8 ANISOU 778 CG GLU 116 2425 2638 4139 -467 -2375 13 9 ANISOU 778 CG GLU 116 2425 2638 4139 -467 -2375 19 9 ANISOU 779 CD GLU 116 2425 2638 4139 -467 -2375 19 9 ANISOU 779 CD GLU 116 2425 2638 4139 -467 -2375 19 9 ANISOU 780 CEI GLU 116 2425 2703 4107 -5100 -739 15 0 9 ANISOU 781 COE GLU 116 2425 2703 4107 -5100 -739 15 0 9 ANISOU 782 N ARG 117 -5.549 35.571 47.300 22.10 -739 15 0 9 ANISOU 783 CA ARG 117 -2.060 35.774 47.040 22.10 -739 15 0 9 ANISOU 784 C ARG 117 -2.060 35.774 47.000 20.60 37.79 10 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0			115 2369		2462
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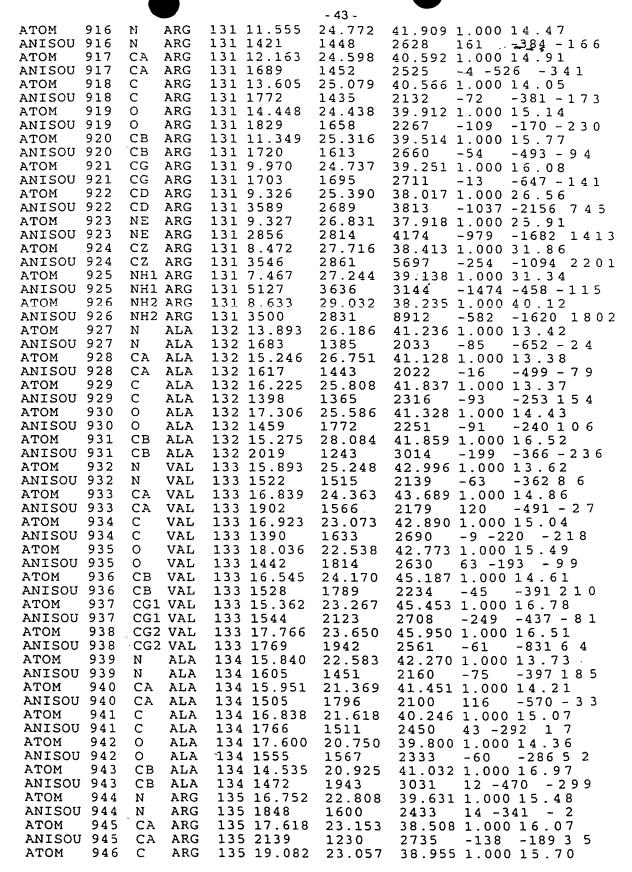


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ANISOU 819 CB THR 120 1951 2204 2720 28 -93 3 4 5 ATOM 820 OG1 THR 120 -3.773 32.238 44.284 1.000 20.49 ANISOU 820 OG1 THR 120 1807 2801 3179 59 -363 5 5 8 ATOM 821 CG2 THR 120 -1.919 32.803 42.933 1.000 22.46 ANISOU 821 CG2 THR 120 2438 3266 2830 475 118 7 0 5 ATOM 822 N GLN 121 0.094 33.708 45.956 1.000 18.62 ANISOU 822 N GLN 121 2180 1657 3237 123 -94 2 1 3 ATOM 823 CA GLN 121 1.466 34.232 45.993 1.000 18.15 ANISOU 823 CA GLN 121 2077 1698 3119 77 96 5 2 0									
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ATOM 822 N GLN 121 0.094 33.708 45.956 1.000 18.62 ANISOU 822 N GLN 121 2180 1657 3237 123 -94 2 1 3 ATOM 823 CA GLN 121 1.466 34.232 45.993 1.000 18.15 ANISOU 823 CA GLN 121 2077 1698 3119 77 96 5 2 0									475 118 705
ANISOU 822 N GLN 121 2180 1657 3237 123 -94 2 1 3 ATOM 823 CA GLN 121 1.466 34.232 45.993 1.000 18.15 ANISOU 823 CA GLN 121 2077 1698 3119 77 96 5 2 0									
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			CA						
									8 1.000 17.04

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ANISO	U 824	С	GLN	121 2022	- 40 -		
ATOM	825	ō	GLN	121 3.510	1431	3019	192 234 223
ANISO	U 825	ŏ	GLN	121 3.510	33.047		0 1.000 19.32
ATOM	826	СВ		121 1894	1800	3645	93 246 1 2 9
ANISO	11 826	CB		121 1.490	35.579		5 1.000 22.90
ATOM	827			121 2520	1479	4702	327 -812 2 7 1
ANISO	027	CG		121 2.888	36.159	46.871	1 1.000 27.04
ATOM	828	CG	GLN	121 2949	2062	5262	-346 -400 1 3 2
ANISO		CD		121 3.530	36.511	45.535	5 1.000 31.94
ATOM		CD	GLN	121 3307	2733	6097	983 1031 9 9
	829	OE.	1 GLN	121 4.660	36.085		983 1031 9 9 7 1.000 62.76
ANISO		OE.	1 GLN	121 3009	9570	11267	1758 2366 2029
ATOM	830	NE2	2 GLN	121 2.859	37.306	11201	1758 2366 2029
ANISO			2 GLN	121 6516	7728	6993	1.000 55.89
ATOM	831	N	$\mathtt{TYR}$	122 1.997	32.791		2815 1745 3 2 4 9
ANISO		N	TYR	122 2389	1518	2501	1.000 16.87
ATOM	832	CA	TYR	122 2.795	31.881		71 -161 - 54
ANISOU		CA	TYR	122 2564	1600	2666	1.000 17.97
ATOM	833	С	TYR	122 3.080	30.600	2006	176 -224 - 56
JOSINA	J 833	С	TYR	122 1870	1460	47.909	1.000 16.83
ATOM	834	0	TYR	122 4.224	30.129	3065	-31 -57 -98
ANISOU	834	0	TYR	122 1891	1952	47.823	,
ATOM	835	СВ	TYR	122 2.018		2872	189 -220 1 2 6
ANISOU	835	CB	TYR	122 2526	31.522	49.960	1.000 18.01
ATOM	836	CG	TYR	122 2.753	1821	2495	2 -325 - 55
ANISOU	836	CG	TYR	122 2332	30.619	50.898	
ATOM	837		TYR	122 4.058	1695	2769	255 -147 - 51
ANISOU	837		TYR	122 2883	30.901	51.323	1.000 21.71
ATOM	838	CD3	TYR	122 2883	2101	3267	-257 -913 3 4
ANISOU		CD2	TYR	122 2.107	29.496	51.415	1.000 21.29
ATOM	839	CE1	TYR	122 2428	2026	3634	128 -267 4 6 8
ANISOU		CE1	TYR	122 4.680	30.037	52.212	1.000 21.27
ATOM	840	CET	TYR	122 2681	2045	3356	140 -725 - 210
ANISOU	840	CEZ	TYR	122 2.746	28.637	52.290	1.000 24.50
ATOM	841	CZ		122 3376	1876	4057	-292 -1163 506
ANISOU	8/1	CZ	TYR	122 4.043	28.914	52.675	1.000 22.16
ATOM	842		TYR	122 3161	1881	3379	95 -909 -128
ANISOU	842	ОН	TYR	122 4.699	28.079	53.566	1.000 23.72
ATOM	843	ОН	TYR	122 3471	2398	3142	52 -1005 - 56
ANISOU	043	N	PHE	123 2.074	30.023	47.253	1.000 16.21
ATOM		N	PHE	123 1794	1571	2793	49 -66 - 54
ANISOU	844	CA	PHE	123 2.347	28.843		1.000 15.71
ATOM		CA	PHE	123 1622	1800	2548	34 -142 -103
	845	C	PHE	123 3.378	29.188		1.000 15.96
ANISOU		C	PHE	123 1681	1304	3078	42 90 3
ATOM	846	0	PHE	123 4.276	28.375		1.000 15.47
ANISOU		0	PHE	123 1703	1437	2739	54 14 24
ATOM	847	CB	PHE	123 1.036	28.309		54 14 - 24 1.000 15.07
ANISOU		CB	PHE	123 1460	1364	2904	2000 15.07
ATOM	848	CG	PHE	123 1.241	27.104		209 -148 1
ANISOU		CG	PHE	123 2090	1620	2906	1.000 17.41
ATOM	849	CD1	PHE	123 1.170	25.831		-39 -179 -238
ANISOU		CD1	PHE	123 1680	1439	43.452	1.000 17.41
ATOM	850	CD2	PHE	123 1.490	27.259	3494	72 -119 -255
ANISOU		CD2	PHE	123 1723	2331	43.513	1.000 18.22
ATOM	851	CE1	PHE	123 1.419	2331	2870	-96 -216 - 372
ANISOU		CE1	PHE	123 2112	1766	44.636	1.000 19.15
ATOM	852	CE2	PHE	123 1.722		3397	212 -540 -536
ANISOU	852	CE2	PHE	123 1901	26.144	42.717	1.000 19.63
ATOM	853		PHE	123 1.635	2476	3083	-134 - 261 - 632
ANISOU			PHE	123 1.035	24.868	43.274	1.000 19.40
ATOM	854		ASP	124 3.164	2424	3421	385 -529 - 490
ANISOU	854		ASP	124 3.164	30.304	44.636	1.000 16.86
	-			+44 134/	1466	2992	-23 -110 1 2 4

855 CA ASP 124 4.060 ATOM 30.640 43.544 1.000 17.82 ATUM 855 CA ASP 124 4.060 30.640 43.544 1.000 17.82 ANISOU 855 CA ASP 124 2103 1747 2921 405 =24 314 ATOM 856 C ASP 124 5.490 30.733 44.024 1.000 17.52 ANISOU 856 C ASP 124 6.402 30.733 219 181 94 8 9 ATOM 857 O ASP 124 6.402 30.324 43.317 1.000 17.18 ANISOU 857 O ASP 124 2086 1427 3015 34 181 177 ANISOU 858 CB AASP 124 3.639 31.997 42.942 0.534 21.77 ANISOU 858 CB AASP 124 3475 2089 2706 642 -372 5 9 7 ATOM 859 CG AASP 124 4.381 32.304 41.659 0.534 19.28 ANISOU 859 CG AASP 124 4.381 32.304 41.659 0.534 19.28 ANISOU 860 OD1 AASP 124 2376 1982 2967 173 -553 4 9 5 ATOM 861 OD2 AASP 124 2189 2636 3164 -28 76 2 1 ATOM 861 OD2 AASP 124 5.068 33.348 41.639 0.534 24.96 ANISOU 861 OD2 AASP 124 3681 2052 3752 -296 -1067 8 8 9 ATOM 862 CB BASP 124 3.632 31.975 42.908 0.466 19.67 ANISOU 863 CG BASP 124 2.368 31.975 42.908 0.466 19.67 ANISOU 863 CG BASP 124 2.368 31.975 42.908 0.466 22.78 ANISOU 863 CG BASP 124 2.368 31.975 42.908 0.466 22.78 ANISOU 863 CG BASP 124 2.368 31.975 42.908 0.466 22.78 ANISOU 863 CG BASP 124 2.368 31.975 42.908 0.466 22.78 ANISOU 864 OD1 BASP 124 2.368 31.975 42.908 0.466 22.78 ANISOU 865 OD2 BASP 124 2.368 31.464 -28 77 1.77 1.75 ATOM 864 OD1 BASP 124 2.368 32.70 1889 872 1.77 1.75 ATOM 865 OD2 BASP 124 3.845 3804 3646 1239 -312 16 44 ATOM 865 OD2 BASP 124 3.845 3804 3646 1239 -312 16 44 ATOM 866 N ARG 125 5.669 31 416 45 152 1.000 1.6 C 5 ANISOU 855 CA ASP 124 2103 1747 2921 405 =24 314 ANISOU 865 OD2 BASP 124 3845 3804 3646 1239 -312 1644 ATOM 866 N ARG 125 5.669 31.416 45.153 1.000 16.65 ANISOU 866 N ARG 125 5.869 31.416 45.153 1.000 16.65
ANISOU 866 N ARG 125 1942 1350 3032 276 139 2 7 6
ATOM 867 CA ARG 125 7.038 31.528 45.646 1.000 17.58
ANISOU 867 CA ARG 125 1918 1819 2944 98 177 2 4 1
ATOM 868 C ARG 125 7.662 30.188 45.992 1.000 17.38
ANISOU 868 C ARG 125 1544 1777 3282 -42 40 2 7 3
ATOM 869 O ARG 125 8.841 29.942 45.754 1.000 18.26
ANISOU 869 O ARG 125 1639 1669 3631 -97 91 -23 3 125 1639 125 7.062 125 2219 1669 3631 -97 91 -233 32.468 46.851 1.000 20.45 870 CB ARG ATOM ANISOU 870 CB ARG 2162 3387 -244 450 -274 33.916 46.344 1.000 28.23 2007 5542 147 666 -222 ATOM 871 CG ARG 125 6.860 ANISOU 871 CG ARG 125 3178 ATOM 872 CD ARG 125 6.693 34.891 47.477 1.000 31.76 ANISOU 872 CD ARG 125 3065 2279 6725 -628 1455 -993 ATOM 873 NE ARG 125 6.496 36.221 46.932 1.000 40.81 ANISOU 873 NE ARG 125 3332 2095 10080 -169 1790 -694 ATOM 874 CZ ARG 125 5.970 37.229 47.628 1.000 43.42 ANISOU 874 CZ ARG 125 4531 2891 9076 839 2072 -2072 - 188 ATOM 875 NH1 ARG 125 5.551 37.025 48.866 1.000 38.62 ANISOU 875 NH1 ARG 125 5.858 38.382 47.006 1.000 42.11 ANISOU 876 NH2 ARG 125 5.858 38.382 47.006 1.000 42.11 ANISOU 876 NH2 ARG 125 5319 2652 8030 908 1627 -681 ATOM 877 N GLN 126 6.884 29.282 46.557 1.000 15.28 ANISOU 877 N GLN 126 1876 1527 2404 -70 13 -60 ATOM 878 CA GLN 126 7.376 27.929 46.853 1.000 15.37 ANISOU 878 CA GLN 126 7.376 27.929 46.853 1.000 15.37 ANISOU 879 C GLN 126 1726 1625 2488 -54 -312 2 0 ATOM 879 C GLN 126 1643 1268 2488 -75 -398 7 1 ATOM 880 O GLN 126 1643 1268 2488 -75 -398 7 1 ATOM 880 O GLN 126 1531 1554 2753 -37 -316 5 3 ATOM 881 CB GLN 126 6.356 27.158 47.702 1.000 17.40 ANISOU 881 CB GLN 126 6.356 27.158 47.702 1.000 17.40 ANISOU 881 CB GLN 126 6.356 27.158 47.702 1.000 26.14 ANISOU 882 CG GLN 126 6.336 27.634 49.150 1.000 26.14 ANISOU 882 CG GLN 126 4503 1690 3739 431 1908 -732 ATOM 883 CD GLN 126 5.208 26.998 49.891 1.000 21.95 ANISOU 884 OE1 GLN 126 2957 2670 2713 0 -123 1 0 2 ATOM 884 OE1 GLN 126 2994 5747 7416 -62 -1272 3 1 4 ATOM 885 NE2 GLN 126 5.524 26.003 50.691 1.000 28.32 875 NH1 ARG 125 5.551 37.025 48.866 1.000 38.62 ATOM 7416 -62 -1272 3147

						- 42 -		
ANISO	J 885	NE	2 GLN	12	6 2867	3971	2022	
ATOM	886	N	TYR		7 6.797	27.287	3922	-184 -780 1311
ANISO	J 886	N	TYR	12	7 1629	1438	44.574	1 1.000 14.52
ATOM	887	CA	TYR	12	7 7.039		2448	-41 -373 - 36
ANISOU		CA	TYR	12	7 1563	26.554	43.317	7 1.000 13.93
ATOM	888	C	TYR			1455	2277	-136 -234 150
ANISOU		č	TYR	12	7 8.289	27.091	42.624	1.000 14.54
ATOM	889	Ö			7 1461	1318	2745	24 -195 19n
ANISOU		Ö	TYR	17	7 9.133	26.345	42.140	1.000 14.39
ATOM	890	CB	TYR	12		1580	2277	34 -252 9
ANISOU		CB	TYR	12		26.676	42.435	1.000 14.00
ATOM	891		TYR		7 1510	1549	2258	29 -180 - 70
ANISOU	1 001	CG	TYR		7 5.752	25.795	41.202	1.000 12.33
ATOM	892	CG	TYR	127		1037	2334	-34 -187 4 5
ANISOU		CDI	TYR	127		24.626	41.024	1.000 14.05
ATOM		CDI	TYR	127	7 1810	1158	2371	7 -84 - 8
	893	CDZ	TYR	127	4.837	26.086		1.000 15.71
ANISOU ATOM			TYR	127		1548	2484	55 -513 2 1
	894		TYR		6.382	23.829		1.000 13.10
ANISOU		CEI	TYR	127		999 25		01 -227 -62
ATOM	895	CE2	TYR	127	4.661	25.322		1.000 15.07
ANISOU			TYR		1928	1620	2177	158 -342 1 9 7
ATOM	896	CZ	TYR	127	5.440	24.179		1.000 13.71
ANISOU		CZ	TYR		1617	1348	2245	-146 -106 2 4 6
ATOM	897	ОН	TYR	127	5.337	23.386	37.811	-146 -106 2 4 6 1.000 15.04
ANISOU		ОН	$\mathbf{T}\mathbf{Y}\mathbf{R}$	127	1682	1755	2279	
ATOM	898	N	THR	128	8.467	28.412	42 616	-87 -60 5 3 1.000 14.69
ANISOU		N	THR	128	1813	1324	2446	-154 -217 268
ATOM	899	CA	THR		9.673	28.984	42.011	-154 -217 2 6 8 1.000 14.67
ANISOU		CA	THR		1867	1469	2238	0.0
MOTA	900	С	THR		10.921	28.552	42 736	-98 -32 195 1.000 14.68
ANISOU		С	THR	128	1794	1318	2466	1.000 14.68
ATOM	901	0	THR		11.900	28.166		59 -123 -285
ANISOU		0	THR		1715	1487	2667	1.000 15.45
ATOM	902	CB	THR	128	9.572	30.544	42.069	-259 153 7 1
ANISOU	902	CB	THR	128	2043	1348	2695	1.000 16.02
ATOM	903	OG1	THR	128	8.519	30.849	41 160	-79 59 4 7 9
ANISOU	903	OG1	THR	128	2226	2038	3008	1.000 19.14
ATOM	904	CG2	THR	128	10.835	31.187	3008	195 -23 5 4 5
ANISOU	904	CG2	THR	128	2107	1329	3793	1.000 19.03
ATOM	905	N	ALA		10.933	28.564	3/93	125 311 618
UOZINA		N	ALA	129	1708	1266	24.085	1.000 14.21
MOTA	906	CA	ALA	129	12.108	28.110	2424	-137 -256 -181
NOSINA	906	CA	ALA		1670	1435	44.836	1.000 15.08
MOTA	907	С	ALA		12.389	26.643	2624	-118 -210 - 225
ANISOU	907	С	ALA	129	1706	1299	44.562	1.000 14.37
ATOM	908		ALA	129	13.552	26.238	2457	-159 -203 1 5 7
ANISOU	908	0	ALA	129	1758		44.445	1.000 14.10
ATOM	909		ALA	120	11.887	1464	2137	-5 -244 -148
ANISOU	909		ALA	120	2132	28.313	46.313	1.000 17.08
ATOM	910	N	SER		11.343	1851	2506	-183 -514 -239
ANISOU	910	N	SER	130	1884	25.819	44.553	1.000 14.18
ATOM	911	CA	SER		11.487	1237	2267	-224 -257 1 7 3
ANISOU	911	CA	SER	130	11.40/	24.375	44.351	1.000 15.44
ATOM	912		SER		1840	1219	2807	-115 -135 - 7
ANISOU	912		SER	130	12.072	24.114	42.965	1.000 14.45
ATOM	913		SER	130	1345	1481	2665	78 - 796 - 209
ANISOU	913		SER	130	13.037	23.329	42.807	1.000 14.43
ATOM	914				1327	1382	2773	-74 -246 1 7 2
ANISOU			SER	120	10.120	23.677	44.663	1.000 17.54
ATOM	915		SER		1555	1225	3884	-379 -647 1 2 6
ANISOU			SER		9.268	23.888	43.558	1.000 27.32
	7 1 3	JG	SER	130	2321	3168	4893	11 -1207 865



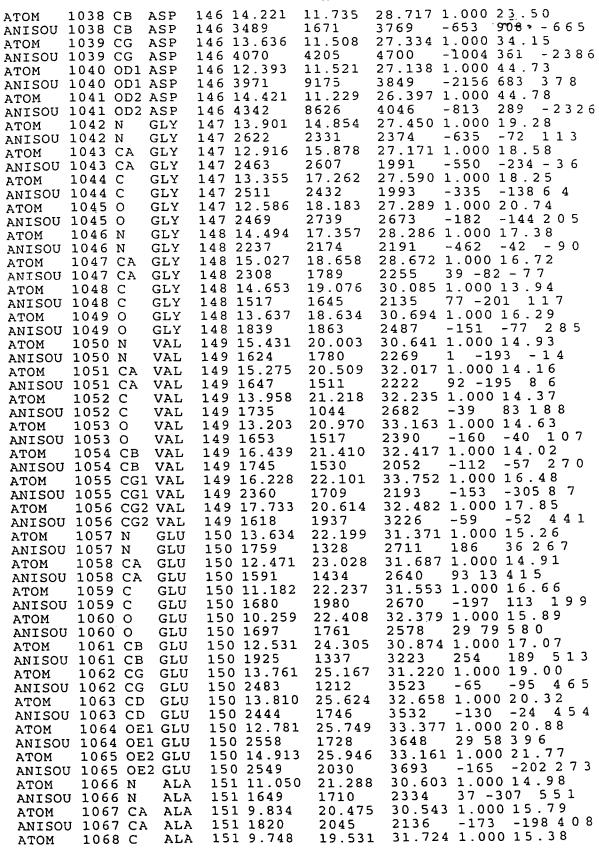
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ANISOU 946	6 C AR	2 125 2050	- 44 -		
ATOM 94			1370	2535	-134 27 121
ANISOU 947	7 O AR			38.176	5 1.000 18 207
ATOM 948			2014	2534	108 256 276
ANISOU 948					1.000 21.96
ATOM 949			1640	2767	-4 -1480 614
ANISOU 949				36.689	1.000 27.53
ATOM 950			2482	2866	816 -610 5 9 5
ANISOU 950				36.393	1.000 23.27
ATOM 951			2428	2865	148 61 1371
ANISOU 951					1.000 22.68
ATOM 952			1575	3556	-116 167 207
ANISOU 952				36.562	1.000 25.90
ATOM 953			2165	3874	921 -506 170
ANISOU 953		135 14.708 135 3582			1.000 23.50
ATOM 954		135 3582	2378	2969	94 137 5 3 2
ANISOU 954		135 13.287	26.758	36.035	1.000 24.30
ATOM 955			2441	3272	-101 72 5 8 2
ANISOU 955	N GLU		23.533	40.149	1.000 15.76
ATOM 956			1696	2396	-178 17 3 1 g
ANISOU 956		136 20.752	23.431	40.694	1.000 15.16
ATOM 957	C GLU	136 21.186	1770	2302	-97 279 140
ANISOU 957	C GLU	136 21.186	22.001	40.978	1.000 16.74
ATOM 958	O GLU	136 22.350	1704	3122	-148 - 172 - 72
ANISOU 958	O GLU	136 22.350	21.637	40.701	1.000 17.42
ATOM 959	CB GLU	136 20.957	1908	2999	7 30 9 2
ANISOU 959	CB GLU	136 20.957	24.284	41.962	1.000 16.64
ATOM 960	CG GLU	136 20.762	1785	2487	53 11 - 16
ANISOU 960	CG GLU	136 2036	25.772	41.718	1.000 17.80
ATOM 961	CD GLU	136 21.534	1714	3014	-286 -169 1 1 n
ANISOU 961	CD GLU	136 2174	26.269 2273	40.513	1.000 20.92
ATOM 962	OE1 GLU	136 22.742	25.987	3503	-343 70 469
ANISOU 962	OE1 GLU	136 2116	23.987	40.454	1.000 24.97
ATOM 963	OE2 GLU	136 21.022	27.037	4938	-494 531 219
ANISOU 963	OE2 GLU	136 2975	2618	39.6/2	1.000 24.77
ATOM 964	N VAL	137 20.262	21.172	3817	-708 -133 1029
ANISOU 964	N VAL	137 1681	1696	2453	1.000 15.34
ATOM 965	CA VAL	137 20.568	19.750		-108 -287 1 1 3
ANISOU 965	CA VAL	137 1755	1802		1.000 15.92
ATOM 966	C VAL	137 20.926	19.086		83 -4 2 1 0
ANISOU 966	C VAL	137 1604	1869	2555	1.000 15.86
ATOM 967	O VAL	137 21.905	18.308		-38 -35 6 6 1 000 1 6 7 8
ANISOU 967 ATOM 968	O VAL	137 1617	2118		1.000 16.70
ATOM 968 ANISOU 968	CB VAL	137 19.358	18.990		72 -151 - 9 0 1.000 15.35
	CB VAL	137 1729	1663	2440	8 -29 5
ATOM 969 ANISOU 969	CG1 VAL	137 19.607	17.478	42 176	1.000 16.93
	CG1 VAL	137 1521	1689	3223	160 -345 9 6
ATOM 970 ANISOU 970	CG2 VAL	137 19.144	19.420	43.724	160 -345 9 6 1.000 15.43
ATOM 971	CG2 VAL	137 1529	2090	2245	-53 -277 1 8 5
ANISOU 971	N LEU	138 20.149	19.407	39.284	1.000 15.52
ATOM 972	N LEU	138 1625	1735	2535	
ANISOU 972	CA LEU	138 20.378	18.881	37.936	-105 -61 109 1.000 15.74
ATOM 973	CA LEU	138 1576	1862	2543	-71 15 5 1
ANISOU 973	C LEU	138 21.721	19.396	37.406	1.000 17.42
ATOM 974	C LEU	138 1588	2119	2912	-87 162 - 45
ANISOU 974	O LEU	138 22.503	18.609	36.846	1.000 19.13
ATOM 975		138 1878	2406	2985	186 317 6 2
ANISOU 975		138 19.211	19.248	36.996	1.000 14.70
ATOM 976		138 1592	1642	2349	-50 141 190
ANISOU 976	CG LEU	138 17.883	18.541	37.375	1.000 14.38
	CG LEO	138 1657	1409		-44 -4 2 8 8
	•				



						- 45 -	
MOTA	977	CD1	LEU	138	16.774	19.122	36.491 1.000 16.13
ANISOU	977	CD1	LEU	138	1743	1848	2539 128 <del>-21</del> 8168
ATOM	978	CD2	LEU	138	17.975	17.027	37.156 1.000 17.48
UOSINA	978	CD2	LEU	138	2185	1435	3021 -107 -480 287
MOTA	979	N	ARG	139	21.963	20.708	37.548 1.000 17.44
ANISOU	979	N	ARG	139	1797	2157	2674 -319 238 192
MOTA	980	CA	ARG	139	23.189	21.319	36.996 1.000 19.06
ANISOU	980	CA	ARG	139	2043	2462	2735 -366 482 376
ATOM	981	С	ARG	139	24.419	20.734	37.685 1.000 19.72
ANISOU	981	С	ARG	139	1797	2600	3097 -518 482 376
MOTA	982	0	ARG		25.461	20.432	37.094 1.000 20.70
ANISOU	982	0	ARG		2046	2469	3350 -288 607 195
ATOM	983	CB	ARG	139	23.152	22.850	37.101 1.000 24.54
ANISOU	983	CB	ARG	139	2525	2403	4396 -402 951 690
ATOM	984	CG	ARG		23.886	23.665	36.073 1.000 36.05
ANISOU		CG	ARG		6517	2967	4212 -2176 1609 1 4 0
ATOM	985	CD	ARG		23.852	25.148	36.443 1.000 44.95
ANISOU	985	CD	ARG		7459	1902	7716 -242 -1324 1930
ATOM	986	ΝE	ARG		22.525	25.727	36.547 1.000 43.27
ANISOU		ΝE	ARG		6637	3846	5959 -828 -2173 -698
MOTA	987	CZ	ARG		21.821	26.330	35.605 1.000 41.34
ANISOU		CZ	ARG		5939	4102	5666 497 645 1140
MOTA	988		ARG		22.308	26.436	34.376 1.000 44.01
ANISOU			ARG		6564	4146	6011 550 1393 3 3 6
ATOM	989		ARG		20.614	26.837	35.833 1.000 45.75
ANISOU			ARG		6162	4618	6602 537 1938 2405
ATOM	990	N	ALA		24.357	20.566	39.009 1.000 18.77
ANISOU		N	ALA		1742	2387	3003 -255 145 6 9
ATOM	991	CA	ALA		25.532	20.169	39.773 1.000 19.53
ANISOU		CA	ALA		1583	2641	3197 -28 38 -668
ATOM	992	C	ALA		25.932	18.732	39.490 1.000 18.96
ANISOU	992	C	ALA		2018	2342	2843 -67 76 -103
ATOM	993	0	ALA		27.109	18.335	39.626 1.000 21.36
ANISOU		0	ALA		1900	2436	3778 -2 472 - 8 0
ATOM	994	CB	ALA		25.273	20.345	41.275 1.000 19.74
ANISOU		CB	ALA		1824	2592	3084 35 0 - 360
MOTA	995	N	THR		24.958	17.943	39.062 1.000 20.32 3498 -115 305 -138
ANISOU		N	THR		2014	2209	3498 -115 305 -138 38.717 1.000 17.15
ATOM	996	CA	THR		25.151 1870	16.530 2039	2609 61 51 2 1 8
ANISOU	997	CA C	THR THR		25.269	16.278	37.208 1.000 17.44
ATOM ANISOU		C	THR		1492	2443	2693 21 278 1 9 9
ANISOU	998	0	THR		25.343	15.106	
ANISOU		0	THR		1871	2623	2814 63 579 - 63
ATOM	999	СВ	THR		24.048	15.629	39.290 1.000 16.79
ANISOU		CB	THR		1708	2261	2410 83 164 3 1
ATOM			THR		22.788	16.012	38.710 1.000 17.18
ANISOU					1894	2235	2399 -101 -53 5 1 8
ATOM			THR		23.982	15.734	40.807 1.000 17.83
ANISOU			THR		1521	2878	2377 164 -43 2 0
ATOM	1002		GLY		25.361	17.301	36.381 1.000 19.69
ANISOU			GLY		2091	2789	2603 -708 302 297
ATOM	1003		GLY		25.517	17.123	34.923 1.000 19.08
ANISOU			GLY		1878	2819	2551 128 -163 2 5 5
ATOM	1004		GLY		24.284	16.441	
ANISOU			GLY		1972	2410	2744 0 252 - 117
ATOM	1009		GLY	142		15.755	33.315 1.000 22.41
ANISOU			GLY	142		2681	3403 -161 571 -680
ATOM	100		THR		3 23.093	16.650	
ANISOU			THR		3 1895	2002	2667 67 300 2 4 4
ATOM		7 CA			3 21.909	15.932	

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	40
ANISOU 1007 CA THR	-46- 143 1953 2006 2456 164 222 -
ATOM 1008 C THR	143 30 20 2456 164 332 6 6
ANISOU 1008 C THR	143 2140 16.660 33.432 1.000 177.70 2
ATOM 1009 O THR	143 2149 1/95 2521 82 196 1 1 7
ANISOU 1009 O THR	33.764 1.000 20 30
ATOM 1010 CB THR	3103 344 12 - 28
THE COURSE THE	143 21.085 15.490 35.623 1 000 16 40
ATOM 1011 OG1 THR	2329 2148 -37 95 - 44
ANISOU 1011 OG1 THR	143 21.922 14.692 36.479 1 000 17 93
ATOM 1012 CG2 THR	2688 -109 39 33 3
ANISOU 1012 CG2 THR	$\frac{143}{19.88}$ / $\frac{14.621}{19.88}$ $\frac{35.270}{1000}$
	3167 -192 -94 100
ATOM 1013 N GLU ANISOU 1013 N GLU	144 20.742 16.070 32.248 1.000 18 79
3.003/	2800 47 12 - 121
ANT COTT A CALL	144 19.729 16.573 31 334 1 000 30 13
3.003/ 101-	7 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
ANISOU 1015 C GLU	144 18.63/ 15.506 31.254 1.000 19 18
ATOM 1016 O GLU	2418 -292 230 -131
33170000	144 18.82/ 14.438 30.665 1 000 21 46 3
	$\frac{2442}{11}$ 3446 19 649 - 8.8
TOTAL CD MGTO	30.006 0.753 29 50
	3566 -855 206 1501
1.010	144 20.195 18.567 29.741 0.753 36 54
	3913 -1729 1760 7 0 5
AGEO	30.426 0.753 33 13
ATOM 1020 OE1AGLU	144 110 3432 4966 104 744 884
ANISOU 1020 OE1AGLU	31.641 0.753 51 91
ATOM 1021 OE2AGLU	4940 -868 -202 - 500
ANISOU 1021 OE2AGLU	144 22.207 19.910 29.807 0.753 50 79
ATOM 1022 CB BGLU	7653 ~3071 3099 ~1240
	14 263 72 16.724 29.951 0.247 18.36
	3016 334 16 2 6 2
ANISOU 1023 CG BGLU	144 1301 17.988 29.779 0.247 23.54
ATOM 1024 CD BGLII	4056 -38 595 558
	144 3500
ATOM 1025 OF 1 BCLII	39/5 5064 438 -20 2031
ANISOU 1025 OE1BGLII	144 2222
ATOM 1026 OF 2 BCLIL	2861 389 1729 1280
ANISOU 1026 OE2BGLU	114 217014 19.464 27.990 0.247 35.35
ATOM 1027 N PRO	5108 35 1752 1516
ANISOU 1027 N PRO	1/5 2122
ATOM 1028 CA PRO	1/5 16 200 14 70 20 02 15 8
ANISOU 1028 CA PRO	145 2290 1040 1.000 17.41
TOTAL TOTAL DBU	2384 -73 400 1 2
ANISOU 1029 C PRO	145 2386 1055
ATOM 1030 O PRO	145 45 45 2573 -110 297 - 107
ANISOU 1030 O PRO	145 2271 2196 2473 1.000 18.26
ATOM 1031 CB PRO	145 45 45 45 45 45 45 45 45 45 45 45 45 4
ANISOU 1031 CB PRO	1/5 2101 100 17.07
ATOM 1032 CG PRO	445 45 45 4 40 4 40 4 4 4 4 4 4 4 4 4 4
ANISOU 1032 CG PRO	146 2241
ATOM 1033 CD PRO	145 48 49 49 49 49 49 49 49 49 49 49 49 49 49
ANISOU 1033 CD PRO	145 2170 1601 12049 1.000 17.54
ATOM 1034 N ASP	2004 1/8 -88 3/13
ANISOU 1034 N ASP	146 2140 1965 2700 18.13
ATOM 1035 CA ASP	146 14 000 = 2730 = 00 321 = 152
ANISOU 1035 CA ASP	146 2487 1664 2853 220 210
ATOM 1036 C ASP	146 13.809 14.154 28 566 1 000 10 07
ANISOU 1036 C ASP	146 2824 1979 2064 31 300 7.00
ATOM 1037 O ASP	146 12.959 14 333 29 422 1 000 10 00
ANISOU 1037 O ASP	146 2491 2173 2222 1.000 18.29
	2173 2287 -168 203 -230



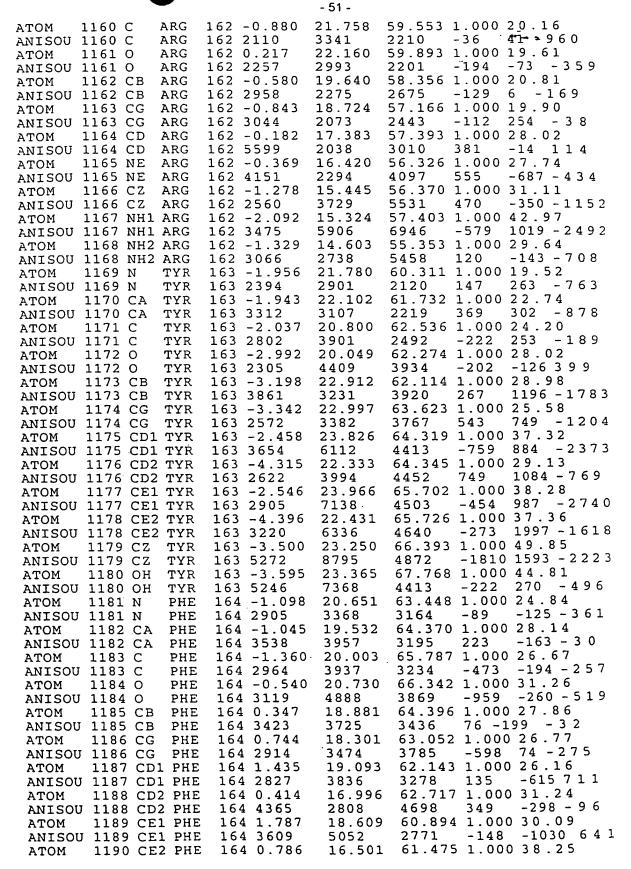
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ANTONIA		- 48 -	
ANISOU 1068 C ALA 1 ATOM 1069 O ALA 1	51 1674	1953	2216 165 181 442
ANTICON TO SE	51 8.642	19.186	
3004	51 1778	1852	2643 - 152 110 330
ANTCOM 1070 -	51 9.823	19.663	29.236 1.000 18 05
ATOM 1071 N PHF 1	51 1910 52 10.893	2811	2139 -275 -316 1 6 6
ANISOU 1071 N PHE 1	52 1858		32.306 1.000 14.25
ATOM 1072 CA PHE 1	52 10.893	1132 18.285	2423 10 -107 263
ANISOU 10/2 CA PHE 1	52 1457	1291	2252
ATOM 10/3 C PHE 1	52 10.406	19.056	2353 -102 -34 3 0 4 34.695 1.000 13.93
AMON 100	52 1481	1400	2412 -43 165 106
ANTCOM 1004	52 9.679	18.495	2412 -43 -165 1 9 6 35.558 1.000 14.50
ATOM 1075 CB PHE 1	52 1590	1482	2438 -85 252 c
ANISOU 1075 CB PHE 10	52 12.309 52 1504		33.728 1.000 13 95
ATOM 1076 CG PHE 1	52 13.475	1547	2248 - 29 111 462
ANISOU 1076 CG PHE 10	52 1747	16.966 1386	35.011 1.000 14.04
ATOM 10// CD1 PHE 15	52 12.032	15.653	2200 88 -58 2 4 7
ANISOU 10// CD1 PHE 15	52 1906	1306	35.076 1.000 13.90 2069 165 -36 281
ANTCOM 1000 CD2 FRE 13	2 13.094	17.499	2069 165 -36 281 36.127 1.000 15.67
	2 1927	1770	2259 -155 -115 2 3 3
ANTICOT AGE	2 12.213	14.949	36.263 1.000 14 06
ATOM 1080 CE2 PHF 15	52 1669 52 13.323	1507	2165 182 - 282 3 4 7
ANISOU 1080 CE2 PHE 15	52 1724	16.799	37.276 1.000 14.83
ATOM 1081 CZ PHF 15	2 12.861	1671 15.522	4240 35 <b>-</b> 112 165
ANISOU 1081 CZ PHE 15	2 1994	1734	37.361 1.000 14.86 1916 -162 99 113
ATOM 1082 N LEU 15	3 10.789	20.324	1916 -162 99 1 1 3
MUISOU 1082 N LEU 15	3 1742	1355	34.789 1.000 15.25 2696 58 110 1 5 4
ANTECOM 1000	3 10.454	21.151	35.939 1.000 14.65
3.0037	3 1783	1429	4354 -66 162nz
ANTECOM 1004	3 9.082 3 1732	21.791	35.877 1.000 14 47
ATOM 1085 0 LEU 15	3 8.581	1402	2362 -80 76 1 1
ANISOU 1085 O LEU 15	3 1940	22.216 1454	36.953 1.000 15.82
ATOM 1086 CB LEU 15	3 11.537	22.224	2616 -313 312 -157
ATOM 1007 CB LEU 15	3 1626	1451	36.165 1.000 16.53 3205 -23 269 -83
AMTCOM 1000 -		21.685	3205 -23 269 -83 36.514 1.000 15.90
7 more 10 Hz 13	3 1893	2013	2135 -33 -186 - 36
	3 13.922 3 1732	22.829	36.614 1.000 18 41
ATOM 1089 CD2 LEU 15	3 1732	2473	2791 -156 80 -876
ANISOU 1089 CD2 LEU 15	3 3083	20.883 3182	37.794 1.000 21.76
ATOM 1090 N ASP 15	4 8.473	21.866	2005 365 261 193
ANISOU 1090 N ASP 15	4 1768	1181	34.708 1.000 14.41 2525 -25 -8 293
ANTCOM 1000 -	4 7.092	22.373	2525 -25 -8 2 9 3 34.553 1.000 15.90
3 00 016	4 1665	1615	2760 -195 27 769
ANTOOM 1000 TO	4 6.216	21.161	34.814 1.000 14.66
ATOM 1093 O ASP 15	4 1859 4 5.995	1304	4409 -92 143 515
ANISOU 1093 O ASP 154	4 2561	20.368	33.889 1.000 17.30
ATOM 1094 CB ASP 15	4 6.923	1455 22.909	2557 -29 314 23A
ANISOU 1094 CB ASP 154	1 1905	2077	33.125 1.000 18.59
ATOM 1095 CG ASP 154	1 5°.461	23.157	3081 124 269 1317
AN1500 1095 CG ASP 154	2029	2531	32.768 1.000 19.87 2990 226 129 1436
777 CO.: 400 - 400 - 104	4.561	23.253	33.639 1.000 19.68
ATOM 1097 OD2 ACD 154	1 1949	2209	3318 92 221 4 9 6
3377000- 10 10 10 10	1 5.207 1 2512	23.189	31.554 1.000 23.73
ATOM 1098 N CVC 156		3475	3029 246 -137 653
> > 7 T T T T T T T T T T T T T T T T T		20.904	36.070 1.000 14.25
		1365	2342 -101 -62 5 4 6

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ATOM	1099	CA	CYS	155	5.418	19.569	36.468	1.000 13.45	
ANISOU	1099		CYS		1608	1346		-191 4°-458	
ATOM	1100		CYS		4.157	19.574		1.000 12.49	
ANISOU	1100		CYS	155	1644	1331		-200 -148 6 2	
ATOM	1101		CYS	155	3.224	20.303	36.941	1.000 14.55	
ANISOU	1101	0	CYS		1633	1492		-122 -111 4 4 2	
MOTA	1102	CB	CYS	155	6.664	18.872		1.000 14.37	
NISOU	1102	CB	CYS		1907	1366		122 -137 2 1 1	
ATOM	1103		CYS		7.265	19.595		1.000 14.99	
	1103		CYS		1561	1821		-74 -98 182	
MOTA	1104		GLU		4.060	18.706		1.000 12.89	
ANISOU			GLU		1575	1379		-130 29 1 9 4	
MOTA	1105		GLU		2.788	18.447		1.000 12.98	
ANISOU			GLU		1508	1311		-210 21 140	
ATOM	1106 1106		GLU		2.987 1414	18.676 1198		1.000 12.34 102 24 204	
	1107		GLU GLU		2.828	17.757		1.000 14.89	
ATOM ANISOU			GLU		1875	1425		-15 -54 442	
ANISOU	1108		GLU		2.278	17.047		1.000 14.48	
ANISOU			GLU		1968	1323		-279 120 8 7	
ATOM	1109		GLU		1.855	17.038		1.000 14.86	
ANISOU			GLU		1894	1526		-120 95 -152	
ATOM	1110		GLU	156	0.523	17.687	36.932	1.000 17.10	
ANISOU	1110	CD	GLU	156	2091	1976		44 -4 1 4 4	
ATOM	1111	OE1	GLU		-0.204	17.967		1.000 17.98	
ANISOU					1811	2155		-35 10 - 355	
MOTA		OE2			0.214	17.990		1.000 20.99	
ANISOU					2854	2419	2704	-386 -516 5 6 2	
ATOM	1113		PRO		3.292	19.893		1.000 12.09	
ANISOU			PRO		1314	1347	1934	12 -48 2 4 9	
ATOM	1114		PRO		3.576	20.121 1696	1924	1.000 13.28 -68 117 147	,
ANISOU ATOM	1114		PRO PRO	157	1425 2.330	19.996		1.000 12.87	
ANISOU			PRO		1236	1737	1916	-214 -47 124	L
ANISOU	1116		PRO		1.192	20.190		1.000 13.73	•
ANISOU			PRO		1286	1717	2214	-190 -17 143	}
MOTA	1117		PRO		4.061	21.580		1.000 13.94	
ANISOU			PRO		1518	1729	2047	-289 -166 2 4 7	7
MOTA	1118	CG	PRO	157	3.363	22.184	41.226	1.000 13.06	
ANISOU	1118	CG	PRO		1558	1518	1887	-32 -158 - 88	3
MOTA	1119		PRO		3.494	21.128		1.000 12.03	
ANISOU			PRO		1521	1081	1968	-2 -7 1 2 1	
ATOM	1120		LEU		2.542	19.738		1.000 13.02	
ANISOU			LEU		1554	1493	1899	-124 148 7 3	
ATOM	1121		LEU		1.438 1465	19.699 1552	1815	1.000 12.72 -126 -14 3 6	
ANISOU ATOM	1122		LEU		1.927	20.389		1.000 12.90	
ANISOU			LEU		1230	1715	1957	-27 -29 - 8	n
ATOM	1123		LEU		2.975	19.977		1.000 14.06	•
ANISOU			LEU		1374	1666	2304	59 -257 -236	
ATOM		4 CB	LEU		1.046	18.244		1.000 13.58	
ANISOU			LEU		1673	1590	1896	-213 57 171	
ATOM		5 CG	LEU	158	0.044	18.030	46.945	1.000 14.84	
ANISOU			LEU	158	3 1471	1774	2396	-16 262 24	2
MOTA			LEU		3 -1.333	18.635		1.000 16.96	
JOSINA			LEU		3 1485	2196	2764	5 -148 -401	
MOTA			LEU		3 -0.142	16.539		1.000 14.98	
ANISOU			2 LEU		3 1976	1820	1897	-390 171 7 9	
ATOM	112		LEU		1.139	21.306		1.000 13.44 43 -87 -119	
ANISOU			LEU		9 1509	1434	2165	1.000 13.39	
MOTA	112	9 CA	LEU	10;	9 1.443	21.963	40.5/1	. 1.000 13.39	

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ANTCON 1100 -		- 50 -	
ANISOU 1129 CA LE	U 159 1438	1555	2005
ATOM 1130 C LE	U 159 0.419	21.49	
ANISOU 1130 C LE	U 159 1336	2034	
ATOM 1131 0 LE	J 159 -0.79	0 21.596	4135 -152 -20s - 3 o
ANISOU 1131 O LET	J 159 1414		3 49.419 1.000 15.09
ATOM 1132 CB LET		1999	2319 90 -131 a n
ANISOU 1132 CB LEG			9 48.394 1.000 15 20
ATOM 1133 CG LEI	J 159 1.484	1447	4639 55 -325 -107
ANISOU 1133 CG LEU		24.320	49.669 1.000 17 11
ATOM 1134 CD1 LEG		1689	2005 363 222 2
ANISOU 1134 CD1 LEU		24.114	50.453 1.000 18.70
ATOM 1135 CD2 LEU		1759	3070 379 60
ANISOU 1135 CD2 LEU		25.801	3070 379 -687 -540 49.291 1.000 21.00
		1535	3526 439 600
ANTECOM CO.		21.107	3526 439 -692 - 382 50.774 1.000 14.37
3.003( 3.00		1709	2000 14.37
MITCON TABLE		20.747	2063 -101 -186 4 7
ANISOU 1137 CA ARG		1990	1 1 2 2 3 6 5 1
ATOM 1138 C ARG	160 0.480	21.501	2217 -64 90 -118
ANISOU 1138 C ARG	160 1557	2158	1.000 13.40
ATOM 1139 O ARG	160 1.639	21.401	2135 -34 -46 -38
ANISOU 1139 O ARG	160 1528	2508	1000 10.32
ATOM 1140 CB ARG			2164 63 41 - 1 n a
ANISOU 1140 CB ARG		19.263	52.227 1.000 16 13
ATOM 1141 CG ARG	160 -0.594	2084	1914 -127 -30 120
ANISOU 1141 CG ARG	160 1963		51.155 1.000 17 17
ATOM 1142 CD ARG	160 1963	1934	2628 -140 -212 - 60
ANISOU 1142 CD ARG	160 -0.672		51.627 1.000 18.16
3 MOM 3 4 4 5	160 2767	1965	2166 125 -330 - 35
XXXXCAT 1140	160 -1.382		50.682 1.000 18.11
λ TO M 1 1 4 4	160 2408	1775	
AMICON 1111 CE ARG	160 -1.221	14.789	2699 -56 -308 2 0 50.581 1.000 16.76
ATOM 1144 CZ ARG	160 2191	1748	2428 -97 55 1 7 4
	160 -0.326	14.192	2428 -97 55 1 7 4
ANISOU 1145 NH1 ARG ATOM 1146 NH2 ARG	160 2306	2012	51.374 1.000 20.55 3491 -26 -4573.05
	160 -1.908	14.095	
ANISOU 1146 NH2 ARG	160 2502	2031	49.689 1.000 19.23 2774 181 -147 - 33.9
ATOM 1147 N PHE	161 -0.469	22.257	
ANISOU 1147 N PHE	161 1604	2120	53.755 1.000 15.36
ATOM 1148 CA PHE	161 -0.209	22.975	2111 -37 -63 -128
ANISOU 1148 CA PHE	161 2173	42.9/5	54.999 1.000 16.25
ATOM 1149 C PHE	161 -1.030	1774	2227 - 71 - 187 - 80
ANISOU 1149 C PHE	161 1980	22.236	56.069 1.000 16.98
ATOM 1150 O PUE	161 2 240	2432	
ANISOU 1150 O PHE	161 1981	22.113	55.948 1.000 20 38
ATOM 1151 CR DUE		J Z J L	<del>44/3 -190 -191 - 7</del> 2
ANISOU 1151 CB PHE	161 -0.683	24.431	54.862 1.000 19 76
7 TOM 1150	161 2065	1903	3540 167 355 -198
AMICOU 1150	161 -0.379	25.259	56.109 1.000 23.61
ANISOU 1152 CG PHE ATOM 1153 CD1 PHE	161 3026	1905	
ATOM 1153 CD1 PHE	161 -1.194	25.304	
ANISOU 1153 CD1 PHE ATOM 1154 CD2 PHE	161 3992	2474	57.228 1.000 28.25 4268 1077 369 -1253
	161 0.807	25.978	
ANISOU 1154 CD2 PHE	161 4015	2483	56.141 1.000 26.62
ATOM 1155 CE1 PHE	161 -0.850	25.992	3616 -130 -927 -106
ANISOU 1155 CE1 PHE	161 6873	2097	58.383 1.000 35.29
ATOM 1156 CF2 PHE	161 1.153	2031	4437 1538 -135 -1399
ANISOU 1156 CE2 PHE	161 4643	26.723	57.258 1.000 33.63
ATOM 1157 CZ PHE	161 0.320	3240	4894 1263 -2085 -1268
ANISOU 1157 CZ PHE	161 6071	26.726	58.363 1.000 36.44
ATOM 1158 N ARC	162 -0.358	4282	3493  1455  -2477  -1044
ANISOU 1158 N ARG	162 2095	21.767	57.130 1.000 17 59
ATOM 1159 CA ARG	162 1 22	2487	2103 -118 -135 - 69
ANISOU 1159 CA ARG	162 -1.072	21.078	58.199 1.000 18.27
CA ANG	162 2769	2414	1758 6 178 - 378
			- · • • • 7 7 8



ANISO	U 1190 C	E2 PHE	164	6659	- 52 -	
ATOM	1191 C	2 PHF		1.494	4077 17.298	3797 -740 -1363 -612
ANISO	U 1191 C	Z PHE		3189	5078	00.588 1.000 32:74
ATOM	1192 N		165	-2.469	19.609	4172 712 -944 - 385
	U 1192 N		165	3876	4009	2.000 30.02
ATOM ANISO	1193 C.	_	165	-2.670	19.813	3751 -1371 344 -508 67.809 1.000 33.09
ATOM	U 1193 C. 1194 C		165	3299	5764	3510 =190 90 22 6
	U 1194 C	PRO	165	-1.459		68.638 1.000 36.32
ATOM	1195 0	PRO PRO	165	3538	5745	4518 664 -191 - 224
ANISO		PRO	165	-0.776 4268		$68.371 \ 1.000 \ 32 \ 94$
ATOM	1196 C	B PRO	165	-3.882	4761	3487 220 501 307
ANISO	J 1196 CI	B PRO	165	3807		68.123 1.000 38 44
MOTA	1197 CC	F PRO	165	-4.635	6924 18.842	38/3 - 765 271 027
ANISOU	J 1197 CC	PRO	165	2595	7020	
ATOM	1198 CI		165	-3.690	19.130	3995 5 688 - 828 65 710 1 000 - 828
ANISOL	J 1198 CI		165	3192	5919	65.710 1.000 33.90 3770 -1149 194 169
	1199 N J 1199 N	LEU	178	7.727	7.453	68.180 1.000 64.52
ATOM	1200 CA	LEU	178	12297	5376	6843 278 -218 3721
	1200 CA	LEU	178	7.629	8.260	66.973 1.000 43 31
$\mathtt{ATOM}$	1201 C	LEU	178	10557	2730	3168 -984 -2921 -126
ANISOU	1201 C	LEU	178	6.159 9239	8.539	66.662 1.000 47.36
ATOM	1202 o	LEU	178	5.314	3530	-2598 - 1186 + 204
	1202 0	LEU	178	11777	7.659 5626	06.796 1.000 56.53
ATOM	1203 CB	LEU	178	8.222	7.582	4076 -4835 1265 -602
ANISOU	1203 CB	LEU	178	11470	3734	65.746 1.000 55.55 5902 -1314 -1197 -1822
ATOM	1204 CG	_	178	9.662	7.092	5902 -1314 -1197 -1822 65.774 1.000 62.34
ATOM	1204 CG	LEU	178 :	10812	5116	
	1205 CD 1205 CD	1 LEU	178 9	9.916	6.185	64.579 1.000 54.23
ATOM	1205 CD	T PEO	178 9	9626	4989	5988 1878 -3799 5 1 1
	1206 CD	2 LEU	170 1	10.633 11265	8.264	65.773 1.000 66 44
ATOM	1207 N	ARG	179	5.879	3454	10526 - 1170 4090 - 516
ANISOU	1207 N	ARG	179 7	7.673	9.751 3826	66.192 1.000 52.90
ATOM	1208 CA	ARC	179 4	1.495	10.033	8444 102 1230 1031
ANISOU	1208 CA	ARG	179 7	7235	4820	65.807 1.000 51.26 7421 -229 1890 -383
ATOM	1209 C	ARG	179 4	.242	9.563	7421 -229 1890 -383 64.383 1.000 55.25
ANISOU ATOM	1209 C	ARG	179 7	7178	6083	7731 -946 2260 -1134
ANISOU	1210 0	ARG	179 3	3.120	9.211	64 021 1 000 50 51
ATOM	1210 CB	ARG ARG	179 7	036	7628	7565 -1820 3675 2051
ANISOU	1211 CB	ARG	179 4	.180	11.512	66.040 1.000 41 49
ATOM	1212 CG	ARG	179 6 179 3	202	4440	4/10 -155 1916 1127
ANISOU	1212 CG	ARG	179 6	120	11.700	67.277 1.000 43.15
ATOM	1213 CD	ARG	179 1	888	5908 12.059	4367 90 1338 530
ANISOU	1213 CD	ARG	179 6	180	7453	66.833 1.000 47.63
ATOM	1214 NE	ARG	179 1	.459	13.367	4463 195 860 -531
ANISOU	1214 NE	ARG	179 7	384	7834	67.269 1.000 52.00 4539 1669 -1168 -538
MOTA	1215 CZ 1215 CZ	ARG	179 1	.322	14.470	4539 1669 -1168 -538 66.556 1.000 64.81
ATOM	1215 CZ 1216 NH1	ARG	179 1	0838	8000	5788 1457 -1107 6 3
	1216 NH1	ARG	179 1		14.518	65.268 1.000 59.74
ATOM	1217 NH2	ARC	179 9		0090	5074 3628 -2691 445
ANISOU	1217 NH2	ARG	179 0 179 1		15.606	67.117 1.000 65.83
ATOM	1218 N		180 5	301	2002	5478 4171 -776 1200
ANISOU	1218 N		180 5		9.501 3769	63.589 1.000 43.96
ATOM	1219 CA	MET	180 5			7550 705 852 -1245
ANISOU	1219 CA	MET	180 2	356		62.210 1.000 40.44 7543 -398 574 -1482
ATOM	1220 C	MET	180 6	.552	8.258	7543 -398 574 -1482 61.920 1.000 43.91
ANISOU	1220 C	MET	180 2	731		7733 18 320 - 2324
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ATOM 1221 O MET 180 7.629 8.679 62,327 1.000 39.46 ANISOU 1221 CB MET 180 5.129 10.189 61.219 1.000 49.84 ANISOU 1222 CB MET 180 5.129 10.189 61.219 1.000 49.84 ANISOU 1223 CG MET 180 5.339 9.818 59.757 1.000 62.58 ANISOU 1223 CG MET 180 5.339 9.818 59.757 1.000 62.58 ANISOU 1224 SD MET 180 7.280 8911 7.587 -2331 -3353 -50.5 ATOM 1224 SD MET 180 4.622 11.015 58.608 1.000 74.24 ANISOU 1225 CE MET 180 4.501 10.037 57.110 1.000 79.59 ANISOU 1225 CE MET 180 4.501 10.037 57.110 1.000 79.59 ANISOU 1226 N ALA 181 3523 5646 5055 -271 882 -11132 ATOM 1227 CA ALA 181 3980 3980 62.505 5.271 882 -1132 ATOM 1228 C ALA 181 2975 3842 51.000 37.40 ANISOU 1228 C ALA 181 2975 3842 51.000 37.77 ANISOU 1230 CB ALA 181 6.727 4.817 66.620 1.000 42.66 ANISOU 1230 CB ALA 181 6.727 4.817 66.620 1.000 42.66 ANISOU 1231 N PRO 182 9.541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1231 N PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.52 ATOM 1232 CA PRO 182 9.5541 6.137 59.840 1.000 24.58 63 1.400 1.200 24.					- 53 -	
ANTSOU 1221 CB MET 180 2377 5064 7554 -395 9765 -912 ANTSOU 1222 CB MET 180 2749 7966 8223 -452 -1114 7 2 ANTSOU 1223 CG MET 180 2749 7966 8223 -452 -1114 7 2 ANTSOU 1223 CG MET 180 7280 8911 7587 -2331 -3353 -505 ANTSOU 1224 SD MET 180 7280 8911 7587 -2331 -3353 -505 ANTSOU 1224 SD MET 180 7480 13510 7216 4918 -262 -905 ANTSOU 1225 CE MET 180 7480 13510 7216 4918 -262 -905 ANTSOU 1225 CE MET 180 6119 20000 4120 -1978 1874 -912 ANTSOU 1226 N ALA 181 3523 5646 5055 -271 882 -1112 ANTSOU 1227 CA ALA 181 7.407 6.140 60.986 1.000 37. 40 ANTSOU 1227 CA ALA 181 7.407 6.140 60.986 1.000 37. 40 ANTSOU 1228 C ALA 181 2975 3842 5149 -32 920 9 5 6 ANTSOU 1228 C ALA 181 2973 842 5149 -32 920 9 5 6 ANTSOU 1220 C ALA 181 2903 4021 4765 197 -98 16 4 ANTSOU 1220 C ALA 181 17.834 7.393 8897 1.000 30.77 ANTSOU 1220 C ALA 181 1405 4284 7820 -1023 1629 5 7 ANTSOU 1230 CB ALA 181 4105 4284 7820 -1023 1629 5 5 7 ANTSOU 1231 N PRO 182 9782 4237 2296 -240 -76 3 2 0 ANTSOU 1231 N PRO 182 9782 4237 2296 -240 -76 3 2 0 ANTSOU 1231 N PRO 182 9782 4237 2296 -240 -76 3 2 0 ANTSOU 1231 C ANTSOU	АТОМ	1221 0	MET	180 7.629	8.679	62 327 1 000 39 46
ATOM 1222 CB MET 180 5.129 10.189 61.219 1.000 49.84 ANTISOU 1222 CB MET 180 5.129 749 766 823 -452 -1114 7 2 ATOM 1223 CG MET 180 7.280 891 787 -2331 -3353 -50.5 ATOM 1224 SD MET 180 4.622 11.015 58.608 1.000 74.24 ANTISOU 1224 SD MET 180 4.622 11.015 58.608 1.000 74.24 ANTISOU 1225 CE MET 180 4.501 10.037 57.110 1.000 79.59 ANTISOU 1225 CE MET 180 4.501 10.037 57.110 1.000 79.59 ANTISOU 1226 N ALA 181 6.376 7.112 61.275 1.000 37.44 ANTISOU 1226 N ALA 181 5233 5646 5055 -271 882 -1132 ATOM 1227 CA ALA 181 3900 3980 6250 5-251 882 -1132 ATOM 1227 CA ALA 181 8900 3980 6250 5-252 048 46 1 ANTISOU 1227 CA ALA 181 8900 3980 6250 6-25 2048 46 1 ANTISOU 1229 C ALA 181 2975 3842 5149 -32 920 9 5 6 ATOM 1229 O ALA 181 7.834 7.393 58.997 1.000 30.77 A ANTISOU 1220 CB ALA 181 2975 3842 5149 -32 920 9 5 6 ATOM 1231 N PRO 182 2782 4237 2296 -240 -76 3 2 0 ANTISOU 1231 N PRO 182 2782 4237 2296 -240 -76 3 2 0 ANTISOU 1231 N PRO 182 2782 4237 2296 -240 -76 3 2 0 ANTISOU 1232 CA PRO 182 10.442 6.667 58.820 1.000 9.3.1 ANTISOU 1233 C PRO 182 2612 2870 2326 -335 -117 - 6 5 ANTISOU 1233 C PRO 182 2612 2870 2326 -335 -117 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -117 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 6 5 ANTISOU 1230 CB PRO 182 2612 2870 2326 -335 -17 - 7 - 7 - 7 - 7 - 7 - 7 - 7 - 7 - 7					5064	
ANTSOU 1222 CB MET 180 2749 7966 8223 -452 -1114 7 2 ATOM 1223 CG MET 180 7280 8911 7587 -2331 -3353 -505 ANTSOU 1224 SD MET 180 7480 13510 7216 4918 -262 -905 ANTSOU 1224 SD MET 180 7480 13510 7216 4918 -262 -905 ANTSOU 1225 CE MET 180 6119 20000 4120 -1978 1874 -912 ANTSOU 1226 N ALA 181 3523 5646 5055 -271 882 -1132 ANTSOU 1226 N ALA 181 3523 5646 5055 -271 882 -1132 ANTSOU 1227 CA ALA 181 7.407 6.140 60.986 1.000 37 .40 ANTSOU 1228 C ALA 181 3890 3980 6250 -625 2048 4 6 1 ANTSOU 1229 O ALA 181 2975 3842 5149 -32 920 9 5 6 ANTSOU 1229 O ALA 181 2973 4021 4765 197 -98 1 6 4 ANTSOU 1230 CB ALA 181 4105 4284 7820 -1023 1629 5 5 7 ANTSOU 1231 N PRO 182 2782 4237 2296 -240 -76 3 2 0 ANTSOU 1232 CA PRO 182 2612 2870 2326 -335 -117 - 6 5 ANTSOU 1232 CA PRO 182 2699 2491 2236 -335 -117 - 6 5 ANTSOU 1233 C PRO 182 2699 2491 2236 -335 -117 - 6 5 ANTSOU 1233 C PRO 182 2699 2491 2236 -335 -170 0 24 .68 ANTSOU 1234 O PRO 182 2991 2486 2759 -440 -340 -55 ANTSOU 1234 O PRO 182 2991 2486 2759 -440 -340 -55 ANTSOU 1236 CB PRO 182 11.768 5.351 6.09 -326 -390 178 5 ANTSOU 1236 CB PRO 182 2699 2491 2236 -391 48 -8 6 ANTSOU 1236 CB PRO 182 2899 380 3042 -170 -286 15 3 ANTSOU 1237 CD PRO 182 2899 380 3042 -170 -286 15 3 ANTSOU 1236 CB PRO 182 2899 380 3042 -170 -286 15 3 ANTSOU 1236 CB PRO 182 2899 380 3042 -170 -286 15 3 ANTSOU 1236 CB PRO 182 2899 380 3042 -170 -286 15 3 ANTSOU 1237 CD PRO 182 2899 380 3042 -170 -286 15 3 ANTSOU 1236 CB PRO 182 3552 3582 3863 656 321 10 38 ANTSOU 1237 CD PRO 182 2899 380 3042 -170 -286 15 3 ANTSOU 1236 CB PRO 182 3353 -740 8 1000 24 .65 7 ANTSOU 1237 CD PRO 182 2899 380 3042 -170 -286 15 3 ANTSOU 1236 CB PRO 182 3552 3582 3863 656 8 301 000 35 .36 ANTSOU 1237 CD PRO 182 3353 310 .111 7.414 565 55 .144 1.000 26 .67 7 ANTSOU 1237 CD PRO 182 3353 -150 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -65 5 .301 170 -						
ATON 1223 CG MET 180 5.339 9.818 59.757 1.000 62.58 ANISSOU 1224 SD MET 180 4.622 11.015 58.608 1.000 74.24 50 ANISSOU 1224 SD MET 180 4.622 11.015 58.608 1.000 74.24 50 ANISSOU 1224 SD MET 180 4.622 11.015 58.608 1.000 74.24 50 ANISSOU 1225 CE MET 180 4.501 10.037 57.110 1.000 79.59 ANISSOU 1225 CE MET 180 4.501 10.037 57.110 1.000 79.59 ANISSOU 1226 N ALA 181 8353 5646 5055 -271 882 -1132 ANISSOU 1226 N ALA 181 87.407 6.140 60.986 1.000 37.44 1.000 1227 CA ALA 181 7.407 6.140 60.986 1.000 37.40 1.000 1.						
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ANISOU 1229 O ALA 181 2903	ANISOU		ALA	181 2975	3842	5149 -32 920 956
ANISOU 1229 O ALA 181 2903	MOTA	1229 O	ALA	181 7.834	7.393	58.997 1.000 30.77
ATOM 1230 CB ALA 181 6.727 4.817 60.620 1.000 42.66 ANISOU 1230 CB ALA 181 4105 4284 7820 -1023 1629 5 5 7 ATOM 1231 N PRO 182 9.541 6.137 59.840 1.000 24.52 ANISOU 1231 N PRO 182 2782 4237 2296 -240 -76 3 2 0 ANISOU 1232 CA PRO 182 10.442 6.667 58.820 1.000 20.55 ANISOU 1232 CA PRO 182 2612 2870 2326 -335 -117 - 6 5 ANISOU 1233 C PRO 182 2612 2870 2326 -335 -117 - 6 5 ANISOU 1233 C PRO 182 2609 2491 2236 -391 48 - 8 6 ANISOU 1234 O PRO 182 2991 2486 2759 -440 -340 - 5 5 ANISOU 1235 CB PRO 182 2991 2486 2759 -440 -340 - 5 5 ANISOU 1235 CB PRO 182 2991 2486 2759 -440 -340 - 5 5 ANISOU 1235 CB PRO 182 2589 3860 3042 -170 -286 15 3 ANISOU 1235 CB PRO 182 11.681 5.351 60.393 1.000 24.98 ANISOU 1236 CG PRO 182 3352 3582 3863 60.394 1.000 28.42 ANISOU 1237 CD PRO 182 3352 3582 3863 60.394 1.000 28.42 ANISOU 1237 CD PRO 182 3352 3582 3863 60.394 1.000 28.42 ANISOU 1237 CD PRO 182 3352 3582 3863 60.394 1.000 28.42 ANISOU 1237 CD PRO 182 3352 3582 3863 656 321 1 0 3 8 ANISOU 1237 CD PRO 182 3131 2658 2533 -274 -204 1 7 6 ANISOU 1239 CA HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1239 CA HIS 183 10.749 8.124 54.337 1.000 19.27 ANISOU 1240 C HIS 183 1964 1560 2456 -75 -352 1 2 8 ANISOU 1240 C HIS 183 19.79 27 ANISOU 1240 C HIS 183 19.79 27 ANISOU 1240 C HIS 183 19.749 8.124 54.337 1.000 18.66 ANISOU 1241 O HIS 183 19.355 9.061 54.868 1.000 18.66 ANISOU 1244 NDI HIS 183 19.355 9.061 54.868 1.000 18.66 ANISOU 1244 NDI HIS 183 19.355 9.061 54.868 1.000 18.66 ANISOU 1244 NDI HIS 183 18.39 9.120 55.447 1.000 35.36 ANISOU 1244 NDI HIS 183 3100 2751 4281 262 222 -306 ANISOU 1244 NDI HIS 183 3100 2751 4281 262 222 -306 ANISOU 1244 NDI HIS 183 3100 2751 4281 262 222 -306 ANISOU 1244 NDI HIS 183 3100 37.30 56.980 1.000 35.36 ANISOU 1244 NDI HIS 183 3100 37.30 56.980 1.000 35.36 ANISOU 1244 NDI HIS 183 3100 37.30 56.980 1.000 35.36 ANISOU 1244 NDI HIS 183 3100 37.30 56.980 1.000 35.36 ANISOU 1244 NDI HIS 183 4432 4078 4926 -1190 1466 -1454 4000 1248 N TYR 184 10.890 7.778 56.980 1.000 35.36 ANISOU 1244 NDI HIS 183 4375 3417 757 5	ANISOU	1229 O	ALA	181 2903	4021	4765 197 -98 164
ATOM 1231 N PRO 182 9.541 6.137 59.840 1.000 24.52 ANISOU 1232 CA PRO 182 10.442 6.667 58.820 1.000 20.55 ANISOU 1232 CA PRO 182 2612 2870 2326 -335 -117 - 6 5 ANISOU 1233 C PRO 182 2612 2870 2326 -335 -117 - 6 5 ANISOU 1233 C PRO 182 9.958 6.402 57.408 1.000 19.31 ANISOU 1233 C PRO 182 9.958 6.402 57.408 1.000 19.31 ANISOU 1234 O PRO 182 9.944 55.326 57.080 1.000 21.68 ANISOU 1234 O PRO 182 9.991 2486 2759 -440 -340 - 5 5 ATOM 1235 CB PRO 182 11.768 5.939 59.047 1.000 24.98 ANISOU 1235 CB PRO 182 11.681 5.351 60.393 1.000 28.42 ANISOU 1236 CG PRO 182 11.681 5.351 60.393 1.000 28.42 ANISOU 1236 CG PRO 182 11.681 5.351 60.393 1.000 28.42 ANISOU 1237 CD PRO 182 3352 3582 3863 656 321 10.38 ATOM 1237 CD PRO 182 3333 4905 4000 -826 -390 178 5 ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1239 CA HIS 183 9.757 7.306 55.144 1.000 18.01 ANISOU 1239 CA HIS 183 19.64 1565 252 -341 -455 34 6 ATOM 1240 C HIS 183 1964 1560 2456 -75 -352 12 8 ATOM 1240 C HIS 183 1964 1560 2456 -75 -352 12 8 ATOM 1241 O HIS 183 1970 2173 2945 -136 -243 37 1 ATOM 1242 CB HIS 183 1970 2173 2945 -136 -243 37 1 ATOM 1244 ND1 HIS 183 3.7884 9.362 56.800 1.000 35.36 ATOM 1244 ND1 HIS 183 3.779 10.658 ANISOU 1247 NE2 HIS 183 7.739 10.658 ANISOU 1247 NE2 HIS 183 3.899 9.120 55.447 1.000 35.68 ATOM 1248 CD HIS 183 3.00 2751 428 262 222 -306 ANISOU 1247 NE2 HIS 183 3.899 9.120 55.447 1.000 35.36 ANISOU 1248 CB HIS 183 3.899 9.120 55.447 1.000 35.36 ANISOU 1248 CB HIS 183 3.00 2751 428 262 222 -306 ANISOU 1248 CB HIS 183 3.899 9.120 55.447 1.000 35.36 ANISOU 1248 CB HIS 183 3.837 7.781 54.821 1.000 33.00 16.668 ANISOU 1248 CB HIS 183 3.839 7.778 53.061 1.000 35.36 ANISOU 1248 CB HIS 183 4432 4078 4926 -1190 1466 -1454 ANISOU 1248 CB HIS 183 3.739 10.658 56.980 1.000 35.36 ANISOU 1248 CB HIS 183 4432 4078 4926 -1190 1466 -1454 ANISOU 1248 CB HIS 183 4375 3417 5658 56.980 1.000 35.68 ANISOU 1248 CB HIS 184 410.890 7.778 53.061 1.000 15.68 ANISOU 1248 CB TYR 184 110.572 9.239 51.169 1.000 14.53 ANISOU 1249 CA TYR 184 110.572 9.239 51.169 1.00	MOTA	1230 CB			4.817	60.620 1.000 42.66
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ATOM 1235 CB PRO 182 11.768 5.939 59.047 1.000 24.98 ANISOU 1235 CB PRO 182 2589 3860 3042 -170 -286 1.5 3 ATOM 1236 CG PRO 182 11.681 5.351 60.393 1.000 28.42 ANISOU 1236 CG PRO 182 3352 3582 3863 656 321 10.38 ATOM 1237 CD PRO 182 3333 4905 4000 -826 -390 17.85 ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 9.757 7.306 55.144 1.000 18.01 ATOM 1239 CA HIS 183 1882 2311 2652 -341 -455 3.46 ATOM 1240 C HIS 183 1964 56.561 1.000 18.01 ANISOU 1240 C HIS 183 1964 56.561 54.835 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1242 CB HIS 183 19.64 54.835 1.000 18.66 ANISOU 1242 CB HIS 183 8.388 7.781 54.835 1.000 18.66 ANISOU 1242 CB HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ANISOU 1245 CD2 HIS 183 8.051 ANISOU 1246 CE1 HIS 183 7.789 10.658 ANISOU 1246 CE1 HIS 183 7.789 10.658 ANISOU 1247 NE2 HIS 183 7.829 11.251 55.798 1.000 40.55 ANISOU 1248 N TYR 184 10.890 7.778 ATOM 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.53 ANISOU 1250 C TYR 184 1656 1449 5249 52416 -70 -399 9 8				182 9.958	6.402	57.408 1.000 19.31
ATOM 1235 CB PRO 182 11.768 5.939 59.047 1.000 24.98 ANISOU 1235 CB PRO 182 2589 3860 3042 -170 -286 1.5 3 ATOM 1236 CG PRO 182 11.681 5.351 60.393 1.000 28.42 ANISOU 1236 CG PRO 182 3352 3582 3863 656 321 10.38 ATOM 1237 CD PRO 182 3333 4905 4000 -826 -390 17.85 ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 9.757 7.306 55.144 1.000 18.01 ATOM 1239 CA HIS 183 1882 2311 2652 -341 -455 3.46 ATOM 1240 C HIS 183 1964 56.561 1.000 18.01 ANISOU 1240 C HIS 183 1964 56.561 54.835 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1242 CB HIS 183 19.64 54.835 1.000 18.66 ANISOU 1242 CB HIS 183 8.388 7.781 54.835 1.000 18.66 ANISOU 1242 CB HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ANISOU 1245 CD2 HIS 183 8.051 ANISOU 1246 CE1 HIS 183 7.789 10.658 ANISOU 1246 CE1 HIS 183 7.789 10.658 ANISOU 1247 NE2 HIS 183 7.829 11.251 55.798 1.000 40.55 ANISOU 1248 N TYR 184 10.890 7.778 ATOM 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.53 ANISOU 1250 C TYR 184 1656 1449 5249 52416 -70 -399 9 8				182 2609	2491	2236 -391 48 - 86
ATOM 1235 CB PRO 182 11.768 5.939 59.047 1.000 24.98 ANISOU 1235 CB PRO 182 2589 3860 3042 -170 -286 1.5 3 ATOM 1236 CG PRO 182 11.681 5.351 60.393 1.000 28.42 ANISOU 1236 CG PRO 182 3352 3582 3863 656 321 10.38 ATOM 1237 CD PRO 182 3333 4905 4000 -826 -390 17.85 ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 9.757 7.306 55.144 1.000 18.01 ATOM 1239 CA HIS 183 1882 2311 2652 -341 -455 3.46 ATOM 1240 C HIS 183 1964 56.561 1.000 18.01 ANISOU 1240 C HIS 183 1964 56.561 54.835 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1240 C HIS 183 1964 56.566 1.000 18.14 ANISOU 1242 CB HIS 183 19.64 54.835 1.000 18.66 ANISOU 1242 CB HIS 183 8.388 7.781 54.835 1.000 18.66 ANISOU 1242 CB HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ANISOU 1245 CD2 HIS 183 8.051 ANISOU 1246 CE1 HIS 183 7.789 10.658 ANISOU 1246 CE1 HIS 183 7.789 10.658 ANISOU 1247 NE2 HIS 183 7.829 11.251 55.798 1.000 40.55 ANISOU 1248 N TYR 184 10.890 7.778 ATOM 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR 184 11.605 8.685 52.152 1.000 14.53 ANISOU 1250 C TYR 184 1656 1449 5249 52416 -70 -399 9 8				182 9.448	5.326	57.080 1.000 21.68
ANISOU 1236 CG PRO 182 3352 3582 3863 656 321 1038 ATOM 1237 CD PRO 182 10.215 5.210 60.747 1.000 32.21 ANISOU 1237 CD PRO 182 3333 4905 4000 -826 -390 1785 ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 2131 2658 2533 -274 -204 176 ATOM 1239 CA HIS 183 9.757 7.306 55.144 1.000 18.01 ANISOU 1239 CA HIS 183 1882 2311 2652 -341 -455 3 4 6 ATOM 1240 C HIS 183 10.749 8.124 54.337 1.000 15.74 ANISOU 1240 C HIS 183 1964 1560 2456 -75 -352 128 ATOM 1241 O HIS 183 11.355 9.061 54.868 1.000 18.14 ANISOU 1241 O HIS 183 11.355 9.061 54.868 1.000 18.14 ANISOU 1242 CB HIS 183 8.338 7.781 54.835 1.000 18.66 ANISOU 1242 CB HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1243 CG HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ATOM 1244 ND1 HIS 183 4432 4078 4926 -1190 1466 -1454 ATOM 1245 CD2 HIS 183 4432 4078 4926 -1190 1466 -1454 ATOM 1246 CE1 HIS 183 4375 ATOM 1246 CE1 HIS 183 7.829 11.251 ANISOU 1247 NE2 HIS 183 4375 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184				182 2991	2486	2759 -440 -340 - 55
ANISOU 1236 CG PRO 182 3352 3582 3863 656 321 1038 ATOM 1237 CD PRO 182 10.215 5.210 60.747 1.000 32.21 ANISOU 1237 CD PRO 182 3333 4905 4000 -826 -390 1785 ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 2131 2658 2533 -274 -204 176 ATOM 1239 CA HIS 183 9.757 7.306 55.144 1.000 18.01 ANISOU 1239 CA HIS 183 1882 2311 2652 -341 -455 3 4 6 ATOM 1240 C HIS 183 10.749 8.124 54.337 1.000 15.74 ANISOU 1240 C HIS 183 1964 1560 2456 -75 -352 128 ATOM 1241 O HIS 183 11.355 9.061 54.868 1.000 18.14 ANISOU 1241 O HIS 183 11.355 9.061 54.868 1.000 18.14 ANISOU 1242 CB HIS 183 8.338 7.781 54.835 1.000 18.66 ANISOU 1242 CB HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1243 CG HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ATOM 1244 ND1 HIS 183 4432 4078 4926 -1190 1466 -1454 ATOM 1245 CD2 HIS 183 4432 4078 4926 -1190 1466 -1454 ATOM 1246 CE1 HIS 183 4375 ATOM 1246 CE1 HIS 183 7.829 11.251 ANISOU 1247 NE2 HIS 183 4375 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184				182 11.768	5.939	59.047 1.000 24.98
ANISOU 1236 CG PRO 182 3352 3582 3863 656 321 1038 ATOM 1237 CD PRO 182 10.215 5.210 60.747 1.000 32.21 ANISOU 1237 CD PRO 182 3333 4905 4000 -826 -390 1785 ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 2131 2658 2533 -274 -204 176 ATOM 1239 CA HIS 183 9.757 7.306 55.144 1.000 18.01 ANISOU 1239 CA HIS 183 1882 2311 2652 -341 -455 3 4 6 ATOM 1240 C HIS 183 10.749 8.124 54.337 1.000 15.74 ANISOU 1240 C HIS 183 1964 1560 2456 -75 -352 128 ATOM 1241 O HIS 183 11.355 9.061 54.868 1.000 18.14 ANISOU 1241 O HIS 183 11.355 9.061 54.868 1.000 18.14 ANISOU 1242 CB HIS 183 8.338 7.781 54.835 1.000 18.66 ANISOU 1242 CB HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1243 CG HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ATOM 1244 ND1 HIS 183 4432 4078 4926 -1190 1466 -1454 ATOM 1245 CD2 HIS 183 4432 4078 4926 -1190 1466 -1454 ATOM 1246 CE1 HIS 183 4375 ATOM 1246 CE1 HIS 183 7.829 11.251 ANISOU 1247 NE2 HIS 183 4375 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184 10.890 7.778 53.061 1.000 14.81 ANISOU 1249 CA TYR 184				182 2589	3860	3042 -170 -286 1 5 3
ATOM 1237 CD PRO 182 10.215 5.210 60.747 1.000 32.21 ANISOU 1237 CD PRO 182 3333 4905 4000 -826 -390 1785 ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 2131 2658 2533 -274 -204 176 ATOM 1239 CA HIS 183 9.757 7.306 55.144 1.000 18.01 ANISOU 1239 CA HIS 183 10.749 8.124 5652 -341 -455 346 ATOM 1240 C HIS 183 10.749 8.124 54.337 1.000 15.74 ANISOU 1240 C HIS 183 1964 1560 2456 -75 -352 128 ATOM 1241 O HIS 183 11.355 9.061 54.868 1.000 18.14 ANISOU 1241 O HIS 183 8.338 7.781 54.868 1.000 18.66 ANISOU 1242 CB HIS 183 8.338 7.781 54.855 1.000 18.66 ANISOU 1243 CG HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1243 CG HIS 183 3100 2751 4281 262 222 -3 06 ATOM 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ANISOU 1245 CD2 HIS 183 8.051 10.311 54.821 1.000 33.00 ANISOU 1245 CD2 HIS 183 8.051 10.311 54.821 1.000 35.36 ANISOU 1246 CE1 HIS 183 7.739 10.658 56.980 1.000 35.91 ANISOU 1247 NE2 HIS 183 7.739 10.658 56.980 1.000 35.91 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1249 CA TYR 184 10.572 9.239 51.169 1.000 14.53 ANISOU 1249 CA TYR 184 10.572 9.239 51.169 1.000 14.53 ANISOU 1250 C TYR 184 10.572 9.239 51.169 1.000 14.53				182 11.681	5.351	60.393 1.000 28.42
ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27  ANISOU 1239 CA HIS 183 2131 2658 2533 -274 -204 1 7 6  ATOM 1239 CA HIS 183 9.757 7.306 55.144 1.000 18.01  ANISOU 1239 CA HIS 183 1882 2311 2652 -341 -455 3 4 6  ATOM 1240 C HIS 183 19.749 8.124 54.337 1.000 15.74  ANISOU 1240 C HIS 183 19.64 1560 2456 -75 -352 1 2 8  ATOM 1241 O HIS 183 11.355 9.061  ANISOU 1241 O HIS 183 2297 2093 2504 -509 -127 -1 3 5  ATOM 1242 CB HIS 183 8.338 7.781 54.835 1.000 18.14  ANISOU 1242 CB HIS 183 1970 2173 2945 -136 -243 3 7 1  ATOM 1243 CG HIS 183 8.089 9.120 55.447 1.000 26.67  ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36  ANISOU 1244 ND1 HIS 183 4432 4078 4926 -1190 1466 -1454  ATOM 1245 CD2 HIS 183 8.051 10.311 54.821 1.000 35.36  ANISOU 1246 CE1 HIS 183 4117 2522 5898 1687 -677 -1 7 3  ATOM 1246 CE1 HIS 183 7.739 10.658 56.980 1.000 35.91  ANISOU 1247 NE2 HIS 183 7.829 11.251 55.798 1.000 40.55  ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68  ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68  ANISOU 1248 N TYR 184 1973 1551 2434 -124 -470 1 0 7  ATOM 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68  ANISOU 1249 CA TYR 184 1798 1392 2438 147 -312 1 4 5  ATOM 1250 C TYR 184 10.572 9.239 51.169 1.000 14.53  ANISOU 1250 C TYR 184 10.572 9.239 51.169 1.000 14.53  ANISOU 1250 C TYR 184 10.572 9.239 51.169 1.000 14.53						
ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27  ANISOU 1239 CA HIS 183 2131 2658 2533 -274 -204 1 7 6  ATOM 1239 CA HIS 183 9.757 7.306 55.144 1.000 18.01  ANISOU 1239 CA HIS 183 1882 2311 2652 -341 -455 3 4 6  ATOM 1240 C HIS 183 19.749 8.124 54.337 1.000 15.74  ANISOU 1240 C HIS 183 19.64 1560 2456 -75 -352 1 2 8  ATOM 1241 O HIS 183 11.355 9.061  ANISOU 1241 O HIS 183 2297 2093 2504 -509 -127 -1 3 5  ATOM 1242 CB HIS 183 8.338 7.781 54.835 1.000 18.14  ANISOU 1242 CB HIS 183 1970 2173 2945 -136 -243 3 7 1  ATOM 1243 CG HIS 183 8.089 9.120 55.447 1.000 26.67  ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36  ANISOU 1244 ND1 HIS 183 4432 4078 4926 -1190 1466 -1454  ATOM 1245 CD2 HIS 183 8.051 10.311 54.821 1.000 35.36  ANISOU 1246 CE1 HIS 183 4117 2522 5898 1687 -677 -1 7 3  ATOM 1246 CE1 HIS 183 7.739 10.658 56.980 1.000 35.91  ANISOU 1247 NE2 HIS 183 7.829 11.251 55.798 1.000 40.55  ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68  ANISOU 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68  ANISOU 1248 N TYR 184 1973 1551 2434 -124 -470 1 0 7  ATOM 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68  ANISOU 1249 CA TYR 184 1798 1392 2438 147 -312 1 4 5  ATOM 1250 C TYR 184 10.572 9.239 51.169 1.000 14.53  ANISOU 1250 C TYR 184 10.572 9.239 51.169 1.000 14.53  ANISOU 1250 C TYR 184 10.572 9.239 51.169 1.000 14.53				182 10.215	5.210	60.747 1.000 32.21
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ANISO ATOM			TYR		1717	1383	2916	-103	-443 1 5 0
ANISO	125 125	2 CB	•	184	12.699				0 1-5-46
ATOM		Z CB 3 CG			1686	1323	2943	69 – 1	366 - 1 6 B
ANISO	J 125	3 CG	TYR TYR		12.383		50.562	2 1:00	0 14.85
ATOM	125	4 CD	1 TYR		1743 12.200	1313	2586	109	-567 4 3
ANISO	J 125	4 CD	1 TYR		1549	5.540 1315	51.185	1.000	0 15.49
ATOM	125	5 CD:	2 TYR		12.329	6.836	3021	-29	-575 1 9 0
ANISO	J 125	5 CD:	2 TYR		1724	1763	2552	1.000	15.89
ATOM	125	6 CE	1 TYR	184	11.962	4.396		22 - 22	27 - 64 0 15.61
ANISO ATOM	J 1251	b CE	LTYR		1695	1244	2992	229	-137 1 1 3
ANISO	125 1251	/ CE.	2 TYR	184	12.130	5.661	48.447	1.000	) 17.52
ATOM	125	B CZ	TYR		2340	1776	2540	4 83	3 - 9 0
ANISOU	J 1258	3 CZ	TYR		11.915 1695	4.449	49.083	1.000	16.96
ATOM	1259	но е	TYR		11.682	1736 3.325		-156	-480 3 4
ANISOU	1259	9 он	TYR	184	2020	1775	48.310 3352	1.000	18.81
ATOM	1260		ASP	185	10.924	10.330	50 502	260	-277 - 312 14.36
ANISOU ATOM			ASP	185	1518	1599	2338	87 -2	25 276
ANISOU	1261	L CA	ASP		10.026	11.005		1.000	13.88
ATOM	1262	CA	ASP ASP	185		1322	2078	141	-364 - 42
ANISOU	1262	2 C	ASP	185	10.240 1182	10.490	48.152	1.000	12.57
ATOM	1263	8 0	ASP		11.357	1385 10.135	2211	-160	-77 -130
ANISOU			ASP	185	1177	1637	47.824 2559	1.000	14.14
ATOM	1264	CB	ASP	185	10.294	12.521	2339 49 580	-135	146 140 14.97
ANISOU ATOM	1264	CB	ASP	185	1879	1293	2517	121	-186 <b>-</b> 159
ANISOU	1265	CG	ASP	185	9.702	13.155		1.000	17.61
ATOM			ASP ASP	185	2680	1659	2351	232	-13 - 172
ANISOU	1266	001	ASP	105	9.507 3553	12.466	51.856	1.000	23.69
$\mathtt{ATOM}$	1267	OD2	ASP	185	9.174	3133 14.257	2314	443	-302 5 2 1
ANISOU	1267	OD2	ASP	185	4063	14.257	50.742 3449	1.000	
ATOM	1268	N	LEU	186	9.141	10.465	47.382	644	1140 - 16
ANISOU	1268	N	LEU	186	1271	1378	2126	-117	-117 - 117
ATOM ANISOU	1269 1269	CA	LEU	186	9.169	10.091	45.986	1.000	12 92
ATOM	1270	CA	LEU LEU	186	1533	1225	2150	-331	-84 -175
ANISOU		Č	LEU	106	9.134 1730	11.292	45.052	1.000	14.12
ATOM	1271	Õ	LEU	186	8.971	1307	2330	-93	-165 5 5
ANISOU	1271	0	LEU		3721	11.173 1643	43.849	1.000	20.12
ATOM	1272	СВ	LEU		8.040	9.106	2280 45.609	-423	99 9 2
ANISOU	1272	CB	LEU	186	1509	1310	2393	-270	-375 - 6
ATOM ANISOU	1273	CG	LEU	186	8.020	7.811	46.438	1.000	15 02
ATOM	1273 1274	CD1	LEU	186	1549	1141	3361	-145	-307 1 6 8
ANISOU	1274	CDI	LEU	106	6.929 1686	6.908	45.866	1.000	19.36
ATOM	1275	CD2	LFII		9.369	1845	3825	-700	-209 3 9 6
ANISOU	1275	CD2	LEU	186	1689	7.115 1742	46.341	1.000	18.32
ATOM	1276	N	SER		9.286	12.494	3528	200	-432 1 7 9
ANISOU	1276	N	SER	187	1326	1234	45.618 2608	-26	-95 137
ATOM ANISOU	1277	CA	SER	187	9.388	13.734	44.826	1.000	13 22
ATOM	1277 1278	CA	SER	187	1489	1197	2338	-54	-68 2 9
ANISOU	1278	C	SER SER	187	10.736	13.853	44.134	1.000	12.79
ATOM	1279	Õ	SER		1482 11.683	1186	2192	-17	-114 - 90
ANISOU	1279	0	SER	187	1532	13.076 1257	44.356	1.000	14.50
ATOM	1280	CB	SER	187	9.201	14.915	2720 45 811	16 -2	24 - 113
ANISOU	1280	CB	SER	187	1463	1282	45.811 2147	1.000	12.87
ATOM	1281	OG	SER	187	10.296	14.873	46.716	1.000	-154 9 8
ANISOU	1781	OG.	SER	187	1589	1420	2015	-34	-143 2 2 4

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ATOM	1282	N	MET	188	10.898	14.844	43.292	1.000 13.44
ANISOU	1282		MET		1552	1334	2221	-64 <del>-3</del> 4 <sub>3</sub> - 26
ATOM	1283		MET		12.215	15.380		1.000 12.11
ANISOU	1283		MET		1508	1261	1833	29 -60 - 61
MOTA	1284		MET			16.022		
					12.853			1.000 12.78
ANISOU			MET		1563	1156	2136	167 -311 - 42
MOTA	1285		MET		13.896	15.550	44.600	
	1285		MET		1408	1390	2294	116 -264 - 26
MOTA	1286		MET		12.038	16.300		1.000 13.66
ANISOU	1286	CB	MET	188	1565	1501	2123	44 -161 207
ATOM	1287	CG	MET	188	13.296	17.095	41.315	1.000 14.05
ANISOU	1287	CG	MET	188	1697	1595	2046	66 150 1 3 3
ATOM	1288	SD	MET	188	14.600	15.971		1.000 14.96
ANISOU	1288	SD	MET		1565	1591	2529	109 -81 110
ATOM	1289		MET		16.005	17.102	40.686	
ANISOU			MET		1852	2032	2855	-242 505 121
ATOM	1290		VAL		12.244	17.112		1.000 12.62
ANISOU	1290		VAL		1586	1203	2007	103 -147 - 134
ATOM	1291		VAL		12.565	17.671		1.000 12.60
ANISOU					1412	1438		
			VAL				1937	-228 -11 - 44
ATOM	1292		VAL		11.285	17.968		1.000 11.71
ANISOU			VAL		1328	1294	1825	-170 -171 - 4 9
ATOM	1293		VAL		10.227	18.099		1.000 12.56
ANISOU		_	VAL		1446	1291	2036	21 -320 - 49
MOTA	1294		VAL		13.440	18.955		1.000 12.95
ANISOU			VAL		1150	1517	2252	-174 -205 9 4
MOTA	1295				14.778	18.637	45.167	1.000 15.54
ANISOU	1295	CG1	VAL	189	1376	2094	2437	-140 161 9 1
ATOM	1296	CG2	VAL	189	12.730	20.056	45.082	1.000 15.00
ANISOU	1296	CG2	VAL	189	1763	1391	2547	-130 -483 8 1
ATOM	1297	N	THR	190	11.425	18.067		1.000 12.18
ANISOU	1297	N	THR		1445	1422	1760	-109 -130 1 0
ATOM	1298		THR		10.353	18.454		1.000 11.98
ANISOU			THR		1292	1356	1903	-57 -221 - 151
ATOM	1299		THR		10.879	19.630	49.710	
ANISOU	1299		THR		1178	1436	2124	-32 -297 - 232
ATOM	1300		THR		11.959	19.523	50.320	
	1300		THR		1424	1767	2531	46 -571 -446
ATOM	1301		THR		9.913	17.297	49.808	
ANISOU			THR		1509	1605	1886	-168 80 -121
ATOM	1302				9.481	16.201		1.000 14.47
ANISOU					1693	1469	2334	-100 -25 -194
ATOM	1303				8.778	17.723		1.000 14.79
ANISOU					1696	1510	2415	73 258 - 89
ATOM	1304		LEU		10.148	20.724	49.732	1.000 12.97
ANISOU			LEU		1329	1449	2149	23 -21 - 286
MOTA	1305		LEU		10.511	21.908	50.526	1.000 13.75
ANISOU	1305	CA	LEU	191	1543	1442	2238	78 -206 - 301
ATOM	1306	С	LEU	191	9.603	21.964	51.763	1.000 14.47
ANISOU	1306	С	LEU	191	1543	1689	2265	83 -179 -412
MOTA	1307	0	LEU		8.370	21.868	51.645	
ANISOU			LEU		1517	2486	2297	219 -176 - 725
MOTA	1308		LEU		10.398	23.212	49.722	
ANISOU			LEU		1717	1444	2680	58 -106 -189
ATOM	1309		LEU			23.578	48.973	
ANISOU			LEU		1747	1688	2680	-128 -113 -135
ATOM	1310				12.069	22.565	47.906	
ANISOU					2034	2093	2209	-23 -64 1 9
ATOM			LEU		11.570	24.959		1.000 18.53
ANISOU					. 2297			
ANISOU	1312		ILE		10.199	1906	2837	-345 -437 1 4 8
AION	1312	14	1116	174	. 10.133	22.148	34.340	1.000 15.36

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ANISO			ILE		2 1479	2152	2204	-47	-165 - 164
ATOM	131	CA	ILE		9.417	22.162			) <del>1</del> 5,13
ANISOU ATOM			ILE	192	2 1456	2043	2251	-304	-173 - 280
ANISO	1314 J 1314		ILE	192	9.692	23.423		1,000	1,3-280
ATOM	1319		ILE		1696	1973	2251	-199	-254 - 226
ANISOU	1 1 2 1 2	. 0	ILE		10.836	23.691	55.381		17.20
ATOM	1316		ILE	192		2449	2229	-307	-341 - 574
ANISOU	11316	CB	ILE ILE	192	9.722	20.920	55.040	1.000	17.03
ATOM	1317	. CG1	LILE	192	2 2246 2 9.454	1958	2266	-52	325 - 303
ANISOU	1317	CG1	ILE		3040	19.596 2010	54.317		19.80
MOTA	1318	CG2	ILE		8.995	20.967	2473	-71	128 - 382
ANISOU	1318	CG2	! ILE	192	2278	2354	2262	1.000	18.14
ATOM	1319	CD1	ILE	192	9.420	18.387	55 235	229	290 - 258 31.57
ANISOU	1319	CD1		192	4658	2114	5222	-398	31.57
ATOM	1320	N	GLN	193	8.625	24.172	55.249		-1094 765 17.04
ANISOU ATOM	1320	N	GLN	193	2042	2185	2248	112	-388 - 301
ANISOU	1321	CA	GLN	193	8.680	25.291	56.201	1.000	17.70
ATOM	1322		GLN GLN	193	1737	2167	2824	-204	-186 - 559
ANISOU	1322		GLN	193	7.898	24.869	57.443	1.000	19.67
ATOM	1323	Ô	GLN	103	1882 7.082	2624	2969	-232	211 -840
ANISOU		Ö	GLN	193	2066	23.942 3843	57.426	1.000	26.60
ATOM	1324	СВ	GLN	193	8.129	26.598	4197	-965	-110 6 2
ANISOU			GLN	193	3070	2388	55.643 3561	1.000	
ATOM	1325	CG	GLN		8.913	27.304	54.559	500	-98 -514
ANISOU			GLN	193	4664	2384	3689	656	
ATOM	1326		GLN		8.338	28.665	54.156	1.000	209 0
ANISOU ATOM			GLN	193	2868	2943	4181	791	3 111
ANISOU	1327	OEI	GLN	193	7.193	28.695	53.688		45.31
ATOM	1328	MES	CLM		2826	7147	7241	-51	-616 3173
ANISOU	1328	NF2	GLM GLM	193	9.080 3609	29.748	54.345	1.000	30.44
ATOM	1329	N	GLN	193	8.241	2588	5368	418	1259 6 9 2
ANISOU	1329	N	GLN	194	2926	25.259 2758	58.645	1.000	
ATOM	1330	CA	GLN	194	7.569	24.793	2690	303	-368 - 83
ANISOU	1330	CA	GLN	194	3144	2617	59.847 2855	82 -23	22.68
ATOM	1331	С	GLN	194	7.275	26.054	60.663	1 000	30 - 150
ANISOU	1331	C	GLN	194	2809	2768	2856	117	-396 - 320
ATOM ANISOU	1332	0	GLN	194	7.889	27.100	60.418	1.000	25 26
ATOM	1332 1333		GLN	194	4041	2877	2679	-313	-21 -411
ANISOU	1333	CB	GLN		8.467	23.943	60.739	1.000	29.21
ATOM	1334	CG	GLN GLN		4493	2707	3899	477	-50 939
ANISOU	1334	CG	GLN	194	9.105 3108	22.735	60.083	1.000	28.80
ATOM	1335		GLN		10.296	3530	4305	576	-121 4 9 4
ANISOU	1335	CD	GLN		2961	22.332	60.962	1.000	
ATOM	1336	OE1	GI.N	194	11.421	5384 22.325	3800	824	359 1075
ANISOU	1336	OE1	GLN	194	2781	4189	60.474	1.000	
ATOM	1337	NE2	GI.N		9.998	22.100	3397	118	133 -249
ANISOU	1337	NE2		194	3540	3958	62.232 3832	989	
ATOM	1338	N	THR	195	6.419	25.891	61.658	1 000	645 800
ANISOU			THR	195	2407	3058	3387	-211	-235 - 720
ATOM ANISOU	1339	CA	THR	195	6.476	26.833			27.14
ATOM	1339	C.A.	THR		3459	3544	3308	25 - 50	0 - 8 9 0
	1340		THR		6.933	25.997	63.958	1.000	26.11
ATOM	1341		THR THR		3825 6.639	2829	3268	558	19 -1247
ANISOU	1341		THR		2973	24.815			28.17
ATOM	1342	СВ	THR		5.149	2916 27.534	4815	481	171 -1030
ANISOU	1342		THR	195	3428	2849	63.069		25.87
					J U	2047	3551	-16	-592 -1137



1343 OG1 THR 195 4.111 26.550 63.196 1.000 25.45 ANISOU 1343 OG1 THR 195 3427 3101 3141 -9 -11-7 -7 5 ATOM 1344 CG2 THR 195 4.788 28.396 61.847 1.000 31.31 -9 -1<del>1-</del>7-,-750 ANISOU 1344 CG2 THR 195 4965 2552 4380 274 -70 - ATON 1345 N PRO 196 7.604 26.587 64.923 1.000 30.84 -70 -409 196 7.604 196 5225 3191 196 8.101 25.823 196 3113 3700 196 7.018 25.534 25.823 66.065 1.000 28.50 3700 4016 -279 -443 ANISOU 1345 N PRO 785 -517 -1542 ATOM 1346 CA PRO ANISOU 1346 CA PRO 4016 -279 -441 -646 25.534 67.096 1.000 28.97 1347 C PRO MOTA ANISOU 1347 C PRO 4102 42 113 -1381 196 6.002 26.229 67.192 1.000 32.32 196 4146 4649 3485 901 -180 -1348 O PRO MOTA 3485 901 -180 -1658 ANISOU 1348 O PRO 196 9.094 26.816 66.694 1.000 29.72 1349 CB PRO MOTA ANISOU 1349 CB PRO 196 3888 3292 4111 -285 -353 -1072 196 8.533 28.174 66.364 1.000 34.87 MOTA 1350 CG PRO ANISOU 1350 CG PRO 196 6285 3575 3390 421 -1326 -133 ATOM 1351 CD PRO 196 7.897 28.035 65.012 1.000 33.20 ANISOU 1351 CD PRO 196 6407 3606 2600 -598 -494 -1031 ATOM 1352 N CYS 197 7.289 40.38 3465 -113 85 -1227 ATOM 1353 CA CYS 197 6.519 24.289 69.126 1.000 31.73 ANISOU 1353 CA CYS 197 6.519 24.289 69.126 1.000 31.73 ANISOU 1354 C CYS 197 6.803 25.412 70.124 1.000 35.58 ANISOU 1355 O CYS 197 4213 4819 4486 -480 1126 -2282 ATOM 1355 O CYS 197 7.917 25.939 70.175 1.000 31.34 ANISOU 1356 CB CYS 197 6.940 22.962 69.767 1.000 35.79 ANISOU 1356 CB CYS 197 5913 4705 2980 284 1566 -1423 ATOM 1357 SG CYS 197 6.553 21.535 68.741 1.000 28.53 ANISOU 1350 CG PRO 196 6285 3575 3390 421 -1326 -1332 197 6.553 21.535 68.741 1.000 28.53 1357 SG CYS MOTA 1357 SG CYS 197 3605 4224 3009 50 -5 -452 1358 N ALA 198 5.771 25.791 70.866 1.000 37.27 ANISOU 1357 SG CYS ATOM ANISOU 1358 N ALA 198 5038 4984 4139 -421 1647 -2070 1359 CA ALA 198 5.983 26.811 71.888 1.000 35.91 ATOM ANISOU 1359 CA ALA 198 6273 4144 3230 910 522 -1230 ATOM 1360 C ALA 198 6.993 26.328 72.921 1.000 44.30 ANISOU 1360 C ALA 198 5998 6138 4696 -193 -199 3 3 ATOM 1361 O ALA 198 7.759 27.127 73.457 1.000 42.85 ANISOU 1361 O ALA 198 5209 6328 4742 7 490 - 555

ATOM 1362 CB ALA 198 4.671 27.231 72.532 1.000 41.70

ANISOU 1362 CB ALA 198 7588 5697 2557 2355 1068 - 721

ATOM 1363 N ASN 199 7.036 25.036 73.225 1.000 34.93 ANISOU 1363 N ASN 199 4027 5975 3270 805 167 - ATOM 1364 CA ASN 199 7.969 24.578 74.264 1.000 33.58 ANISOU 1364 CA ASN 199 3643 6167 2950 -670 -265 - ATOM 1365 C ASN 199 9.352 24.262 73.718 1.000 31.53 167 - 621 24.262 73.718 1.000 31.53 5048 2853 384 -420 2950 -670 -265 -808 199 9.352 199 4077 ASN ANISOU 1365 C -420 -855 1365 C 1366 O ATOM 1366 O ASN 199 10.153 23.667 74.467 1.000 36.33 ANISOU 1366 O ASN 199 4223 5624 3957 -403 -1305 -126 ATOM 1367 CB ASN 199 7.441 23.308 74.929 1.000 36.38 ANISOU 1367 CB ASN 199 4533 5029 4262 859 584 -522 ATOM 1368 CG ASN 199 7.198 22.180 73.952 1.000 31.28 ANISOU 1368 CG ASN 199 4030 4863 2993 882 202 1 202 178 ATOM 1369 OD1 ASN 199 7.743 22.151 72.853 1.000 37.62 ANISOU 1369 OD1 ASN 199 4693 6272 3330 122 728 -728 - 56 1370 ND2 ASN 199 6.393 21.190 74.314 1.000 36.42 1132 - 958 ANISOU 1370 ND2 ASN 199 3508 6251 4078 -13 1371 N GLY 144 -692 GLY ANISOU 1371 N 200 10.920 24.304 71.866 1.000 35.26 1372 CA GLY -317 480 -2400 200 4430 4905 4060 ANISOU 1372 CA GLY 200 11.184 22.886 71.429 1.000 36.83

GLY

1373 C

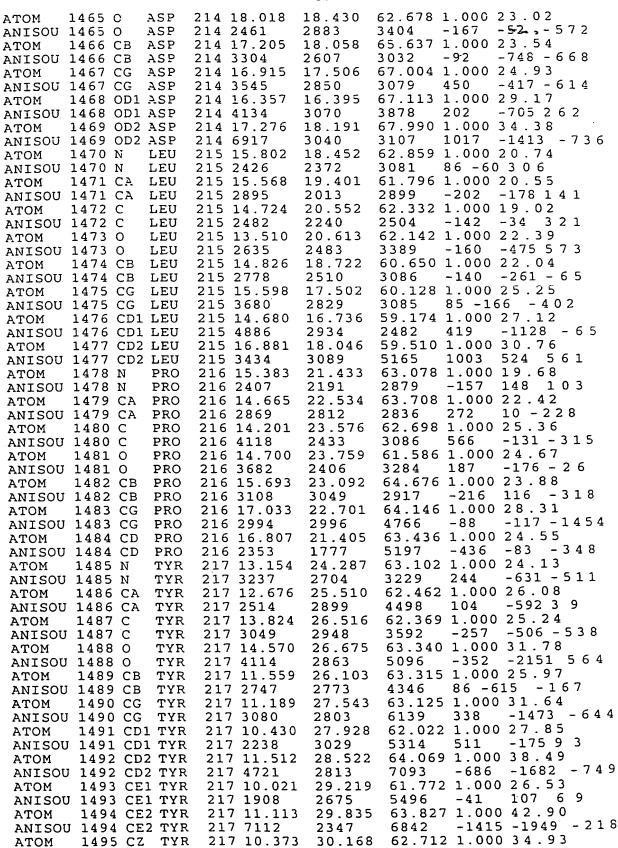
ATOM

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	- 58 -	
ANISOU 1373 C GLY 200	0 4683 4375	
ATOM 1374 0 GLY 200	12.257 22.566	4936 -360 1601 -1460
ANISOU 13/4 O GLY 200	1 2021 4000	- · · · · · · · · · · · · · · · · · · ·
ATOM 1375 N PHE 201	10.264 21.939	
ANISOU 13/5 N PHE 201	3813 4229	2015
ATOM 1376 CA PHE 201	10.491 20.575	204/ 140 400 - 106
ANISOU 13/6 CA PHE 201	3190 4337	2042
ATOM 13/7 C PHE 201	10.752 20.553	
ANISOU 13// C PHE 201	2943 3682	24.09
ATOM 13/8 O PHE 201	9.994 21.255	
ANISOU 13/8 O PHE 201	3583 3184	2055
ATUM 13/9 CB PHE 201	9.250 19.729	3957 10 -421 277 71 413 1 000 2 0
ANISOU 13/9 CB PHE 201	3153 4862	2500 271
ATOM 1380 CG PHE 201	9.425 18 262	3560 -371 -40 - 73 71.027 1.000 34.89
ANISOU 1380 CG PHE 201 ATOM 1381 CD1 PHE 201	4015 4609	
ANTICON ADDITION ZUI	10.395 17.472	71.605 1.000 3 1.18
ANISOU 1381 CD1 PHE 201	3436 4103	4310 -875 -93 -1105
TOTAL CDZ FILE ZUI	8.613 17.681	70.078 1.000 28.84
	2979 4019	3960 329 612 -107
	10.564 16.160	71.240 1.000 37.73
	6489 3608	4239 -1078 -1475 -500
33770077 1007	8.761 16.363	69.679 1.000 31.78
3 MOM 13 0 C = -	4327 3911	3838 652 250 119
NITCON 1201	9.755 15.606	70.265 1.000 29 78
3,000	3705 3397	4211 6 -638 -849
ANTEGOTI 1005	11.706 19.751	69.144 1.000 23 51
3 00 00	2671 3392 11.969 19.626	2868 -292 -1 -57g
3 XT CO!! 1 2 2 -		67.706 1.000 26.37
ATOM 1388 C VAL 202		2946 -667 57 - 72A
ANISOU 1388 C VAL 202	11.423 18.283 2729 3348	67.198 1.000 22.75
ATOM 1389 0 VAI. 202	11.880 17.190	2567 96 -120 -435
MATSON 1388 O AMP 505	3249 3799	67.541 1.000 28.71
ALOM 1390 CB WAT. 202	13.476 19.721	3859 119 31 6 6 1
WITSON 1330 CB AMT 505	3060 3427	67.415 1.000 24.99 3008 -278 283 152
ATUM 1391 CG1 VAL 202	13.715 19.464	3008 -278 283 152
AN 1 500 1391 CG1 VAI, 202	4642 2577	65.938 1.000 27.70 3307 87 1014 - 3
ATOM 1392 CG2 VAL 202	14.050 21 071	3307 87 1014 - 3 67.823 1.000 26.80
ANISOU 1392 CG2 VAL 202	2826 3868	3487 -490 474 -398
NITCON 1	10.405 18 402	66.333 1.000 24.10
1 000	2194 3607	3356 -31 -179 -528
NTTOOM LOUIS CA SER 203	9.634 17 231	65.940 1.000 23.70
3001/ 1000	2373 3584	3046 -290 308 -533
3NT 00 11 1 2 0 3 11 2 0 3	10.168 16.511	64.710 1.000 21.28
3 00 01/	2173 3041	2871 46 227 - 42
DER 203	10.159 15.285	64.640 1.000 27.60
3 m a	4105 3097	3284 -482 1010 - 249
ANTICOM 1300 -	8.148 17.571 2251 3790	65.685 1.000 29.06
ATOM 1398 OG SER 203		5001 -180 203 -2064
117700		66.843 1.000 32.55
ATOM 1399 N 1.FII 204		4231 920 1099 - 382
ANISOU 1399 N LEU 204	^ · ·	63.724 1.000 22.46
ATOM 1400 CA LEI 204		3043 79 450 - 46
ANISOU 1400 CA LEU 204	11.166 16.530 2200 2831	62.544 1.000 20.26
ATOM 1401 C LEU 204	12.595 16.038	2667 45 -18 - 15
ANISOU 1401 C LEU 204	2151 2528	62.747 1.000 18.83
ATOM 1402 O LEII 204	13.443 16.783	2477 -75 60 - 1
ANISOU 1402 O LEU 204	2333 2386	63.251 1.000 20 .47 3059 -303 -195 4 0 4
Arom 1403 CB LEU 204	11.103 17 486	3059 -303 -195 4 0 4 61.362 1.000 21.42
ANISOU 1403 CB LEU 204	2718 2548	7071 344
	<del>-</del>	2871 311 -16 - 8

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ATOM	1404	CG	LEU	204	9.769		61 070	1 000 33 55
ANISOU			LEU		2820	18.188 4319	5617	1.000 33.57 177 1316 1172
ATOM	1405				9.797	18.747		1.000 36.19
ANISOU					4402	3807	5540	1276 -1167 987
ATOM	1406			204	8.581	17.234		1.000 37.76
ANISOU	1406	CD2	LEU	204	3058	5328	5960	-526 -1896 686
ATOM	1407		GLN		12.864	14.836		1.000 20.33
ANISOU			GLN		2518	2644	2563	104 -31 -129
ATOM	1408		GLN		14.209	14.247	62.335	1.000 18.88
ANISOU			GLN		2522	2225	2425	-6 -181 3 6
ATOM ANISOU	1409		GLN		14.512	13.504	61.036	1.000 18.19
ANISOU	1410		GLN GLN		1986 13.577	2383	2543	-143 -188 - 80
ANISOU			GLN		1974	13.033 3063		1.000 19.87
ATOM	1411		GLN		14.296	13.267	2514	-125 -212 -237 1.000 24.25
ANISOU			GLN		3948	2716	2548	202 -343 2 9 6
ATOM	1412		GLN		14.164	13.948		1.000 30.64
ANISOU			GLN		4099	5159	2382	850 -327 - 8 9
ATOM	1413		GLN		14.744	13.078		1.000 28.28
ANISOU			GLN		4473	3633	2640	-161 -1015 -390
ATOM	1414	OEI	GLN		14.307	11.921	66.041	1.000 37.69
ANISOU ATOM					5733	5073	3515	-2145 -699 4 7 8
ANISOU	1415				15.710 6798	13.553	66.711	1.000 40.53
ATOM	1416		ALA		15.752	4417 13.471	4185	-1341 -2865 3 2 3
ANISOU			ALA		2070	2199	2769	1.000 18.52 -240 -13 4
ATOM	1417		ALA		16.152	12.700		-240 -13 4 1.000 18.42
ANISOU	1417	CA	ALA		2074	2351	2575	-100 -158 2 3
ATOM	1418		ALA	206	17.343	11.802		1.000 17.41
ANISOU			ALA		2107	2158	2350	-185 -254 - 17
ATOM	1419		ALA		18.123	12.203		1.000 20.67
ANISOU ATOM	1419		ALA		2469	2410	2973	-48 -711 - 396
ANISOU			ALA ALA		16.637 2119	13.599 2310		1.000 18.77
ATOM	1421		GLU		17.492	10.764	2703	156 -65 1 4 7 1.000 18.09
ANISOU			GLU		2092	2101	2680	-249 -496 - 162
ATOM	1422		GLU		18.710	9.944		1.000 19.48
ANISOU			GLU		2210	2091	3100	-73 -432 - 44
MOTA	1423		GLU	207	19.851			1.000 19.98
ANISOU			GLU		2018	2233	3342	220 -560 5 4 4
ATOM	1424		GLU		19.732	11.068		1.000 20.33
ANISOU			GLU		2000	2753		5 -471 8 9
ATOM ANISOU	1425 1425		GLU GLU		18.566	8.623	58.214	1.000 24.03
ATOM	1425		GLU		3401 19.757	1784	3946	316 -1226 6 1
ANISOU			GLU		3223	7.674 1907	58.295 4121	1.000 24.35 354 93 467
ATOM	1427		GLU		20.730	7.791		354 93 4 6 7 1.000 31.69
			GLU		2729	5178	4134	-1218 -175 1 2 2
ATOM	1428	OE1	GLU		20.376	7.611		1.000 26.97
ANISOU				207	2849	3404	3993	31 -256 309
MOTA	1429	OE2	GLU		21.908	8.121	57.407	1.000 30.70
ANISOU					2484	3416	5764	-233 -342 -1168
ATOM	1430		VAL		20.919	10.936		1.000 18.53
ANISOU ATOM			VAL		2020	2112	2907	130 -362 3 2 0
ANISOU	1431		VAL		22.150	11.547		1.000 19.53
ATOM	1431		VAL VAL		2044 23.341	2238	3137	39 -476 630
ANISOU			VAL	200	23.341	10.755 2792	59.088 3507	
ATOM	1433		VAL		23.460	10.663		225 -461 7 9 7 1.000 23.82
ANISOU			VAL		2262	3240	3547	-40 -858 8 2 5
ATOM	1434		VAL		22.271	13.027		1.000 19.72
								2.000 17.72

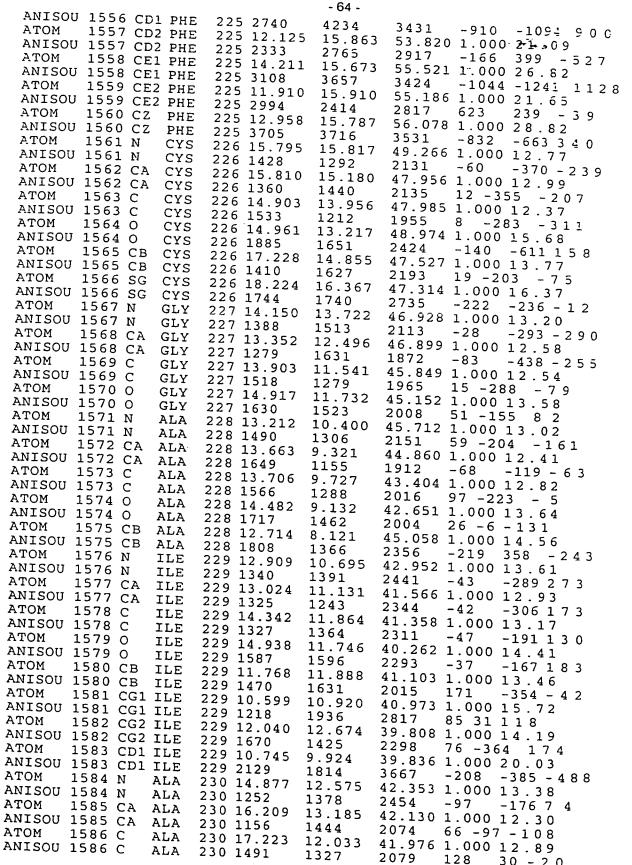
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	1434		VAL	208	1918	2429	3145	-47	-308 3 1 1
ATOM	1435	CG1	VAL	208	23.524	13.626	58.281		-508 3 1 1 - <b>23</b> 2 1 4
ANISOU	1435	CG1	VAL		2524	2374	3895	-202	284 349
ATOM	1436	CG2	VAL	208	21.030	13.812		I.000	19.47
ANISOU	1436				2462	2279	2658	232	-667 - 87
	1437 i 1437 i		GLY		24.180	10,169	58.246		23.88
ATOM	1437 1		GLY		2500	2449	4123	465	-711 3 6
	1438 (		GLY	209	25.306	9.374	58.773	1.000	26.42
ATOM	1439 (		GLY		1987	3599	4450 4,	460	-487 5 1 6
	1439 (		GLY GLY	209	24.905	8.250	59,695	1.000	30.01
ATOM	1440		GLY	209	3469 25.609	3240	4693	238	-1422 732
	1440		GLY	209	4053	7.835	60.629		31.45
ATOM	1441 1		GLY		23.691	4458	3438	1225	-897 8 3
ANISOU	1441 N		GLY	210	3165	7.702 3214	59.523		_
MOTA	1442 (	CA (	GLY	210	23.263	6.585	3744	259	-86 350
	1442 (	CA (	GLY	210	4603	3091	60.360 3619	1.000	
ATOM	1443 (		GLY		22.622	6.993	61.663	~55 1 000	-997 5 8 4
	1443 (		GLY	210	5827	4212	4507	-2536	
ATOM	1444		GLY	210	22.160	6.187	62.481	1 000	732 5 0
	1444		GLY	210	4152	6516	5082	-1874	-567 2346
ATOM	1445 N		ALA	211	22.512	8.274	61.976	1 000	70 / 2346
ANISOU	1445 N	-	ALA		4803	4625	3037	1372	-1177 632
MOTA	1446		ALA	211	21.828	8.603	63.235		35.62
ANISOU	1446		ALA	211	3993	5958	3584	1061	-610 9 7 0
ANISOU	1447 0		ALA	211	20.663	9.543	62.940	1.000	31.43
ATOM	1447 C		ALA		3508	4737	3699	302	69 1854
ANISOU	1448 (	-	ALA		20.652	10.097	61.858	1.000	28.28
ATOM	1449 C		ALA		3661	4062	3020	-571	-551 1010
ANISOU	1449 C	-	ALA ALA	211 711	22.812	9.278	64.170	1.000	41.36
ATOM	1450 N		PHE	211	3644 19.682	8904	3169	1372	-18 -791
ANISOU	1450 N		PHE	212	5211	9.676	63.825	1.000	36.68
ATOM	1451 C		PHE		18.620	4237	4489	1166	1265 2171
ANISOU	1451 C		PHE	212	4490	10.654 3167	63.641		
ATOM	1452 C	F	PHE		19.100	12.023	3293	263	504 1037
ANISOU		F	PHE	212	6746	3760	64.124 2685		
ATOM	1453 O	F	PHE		19.667	12.191	65.210	-248	-539 7 7 6
ANISOU			PHE	212	6144	5384	3335	-549	-1129 1220
ATOM	1454 C		PHE -		17.358	10.219	64.388	1 000	123 1220
ANISOU	_		PHE	212	6376	2569	8288	1348	3748 2314
ATOM	1455 N	T	THR	213	18.906	13.008	63.271		26 30
ANISOU	1455 N		THR	213	4134	2738	3122	662	-581 1 0 0
ATOM	1456 C		THR	213	19.424	14.359	63.433	1.000	25 08
ANISOU			THR		3587	2852	3089	767	-810 - 323
ATOM	1457 C		THR	213	18.190	15.283	63.400	1.000	23.81
ANISOU ATOM	_		THR		2835	2652	3560	215	-855 - 643
ANISOU	1458 0	_	CHR	213	17.329	15.137	62.517	1.000	21.40
ATOM	1458 C		HR	213	2640	2269	3223	-328	-580 -179
ANISOU	1459 C		THR	213	20.398	14.759	62.308	1.000	27.60
ATOM	1460 0	G1 m	HR		3155	3220	4113	189	-356 - 798
ANISOU	1460 0	GI T	אתו סטי	213	21.673	14.084	62.374	1.000	
ATOM	1461 C	G2 m	THE		3582 20.735	4220	4356	746	-410 5 2 0
ANISOU	1461 C	G2 T	HP		4422	16.254	62.355	1.000	
ATOM	1462 N		ASP		18.119	3320	3448	-106	-1265 - 204
ANISOU	1462 N		SP	214	2790	16.177	64.371		
ATOM	1463 C	A A	SP		17.001	2236 17.110	2972	-82	-380 - 142
ANISOU	1463 C		SP	214	2742	2095	64.462	T.000	
ATOM	1464 C	А	SP		16.994	18.030	2993	-117	-898 - 379
ANISOU	1464 C		SP	214	2373	2525	63.226 2923	1.000	
					- · <del>-</del>		4743	182	-169 -237



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ANISO				21	7 4042	2747	6483 -1462 -545 1.6.6
ATOM	149	6 ОН	TYR	217	7 9.996	31.486	
ANISO			TYR	217	7 5499	2895	
ATOM	149		ARG	218	3 14.022	27.110	5439 -753 -250 - 289
ANISO	U 149	7 N	ARG		3461	2406	
ATOM	149	8 CA	ARG		3 14.923	28.243	3852 -227 -533 -476
ANISO	U 1498	B CA	ARG	218	3630		61.049 1.000 29.26
$\mathtt{ATOM}$	1499	9 C	ARG		3030	3270	4219 -784 -1349 260
ANISO	U 1499	9 C	ARG	210	4063	29.336	60.365 1.000 24.81
ATOM	1500		ARG	210	13.746	2949	4415 -382 -228 - 56
ANISO	J 1500	0 0	ARG	210	6298	29.174	59.212 1.000 29.56
ATOM	1501		ARG		16.162	2267	2666 -890 -994165
ANISOU	J 1501	CB	ARG	210	3223	27.823	60.256 1.000 35.90
ATOM	1502	CG	ARG	210	17.369	3685	0/32 - 624 - 703 00c
ANISOU	J 1502	CG	ARG	210	17.369 4740	28.665	60.661 1.000 51.38
ATOM	1503	CD	ARG			6768	8015 -3031 430 -102
ANISOU	J 1503	CD	ARG	210	18.539	28.606	59.701 1.000 38 84
ATOM	1504		ARG	210	4968	6308	3482 - 3596 - 1165 1647
ANISOU	1504	NE	ARG	218	19.343	27.395	59.905 1.000 45.09
ATOM	1505	C7	ARG	218	4655	7495	4982 - 2325 - 962 - 94
ANISOU	1 1505	C 7	ARG	218	20.272	27.208	58.959 1.000 55.53
ATOM	1506	NHI	LARG	218	5299	11458	4340 -2701 -1188 -1948
ANISOU	1506	ועוו	אפכ	218	20.289	28.158	58.031 1.000 60.85
ATOM	1507	MHO	ARG	218	2399	16648	4071 -1943 -1333 548
ANISOU	1507	NHO	DAM	218	21.060	26.165	59.001 1.000 60.37
ATOM	1508	N	PRO	218	8580	10111	4247 - 2152 639 - 4241
ANISOU		NI		219	13.871	30.496	60.972 1.000 25 89
ATOM	1509	CA	PRO PRO	219	2625	4126	3086 35 296 -1014
ANISOU	1509	CA	PRO	219	13.065	31.548	60.326 1.000 28.10
ATOM	1510	CA	PRO	219	2828	3120	4730 -410 379 -696
ANISOU	1510		PRO	219	13.636	31.959	58.981 1.000 28 43
ATOM	1511	0	PRO		3141	3010	4653 -190 116 -328
ANISOU	1511	Õ	PRO	219	12.904	32.393	58.081 1.000 34.17
ATOM	1512		PRO	219	4734	3500	4/50 302 -798 - 893
ANISOU	1512	CB	PRO	219	13.115	32.717	61.316 1.000 39 70
ATOM	1513	CC	PRO		5621	3612	5852 <b>-</b> 500 1615 - 1527
ANISOU	1513	CG	PRO	219	13.368	32.033	62.628 1.000 42 38
ATOM	1514	CD	PRO	219	6139	5277	4688 -257 2084 - 2086
ANISOU	1514	CD	PRO	219	14.370	30.943	62.289 1.000 32 77
ATOM	1515	M	ASP	219	3901	5719	2831 -602 828 -1603
ANISOU	1515	71		220	14.950	31.824	58.811 1.000 25 65
ATOM	1516	C y	ASP	220	3328	1582	4837 -276 801 -878
ANISOU	1516	$C\lambda$	ASP	220	15.590	32.280	57.587 1.000 26 45
ATOM	1517	CA	ASP		3594	2115	4341 -782 248 -861
ANISOU	1517	Č	ASP ASP	220	15.781	31.305	56.451 1.000 28.46
ATOM	1518			220	3549	1843	5423 -111 1638 - 943
ANISOU	1518	0	ASP	220	16.432	31.620	55.433 1.000 25.80
ATOM	1519	CB	ASP	220	3249	2021	4533 -140 623 -412
ANISOU	1519	CB	ASP	220	16.911	32.962	57.998 1.000 33.76
ATOM	1520	CC	ASP	220	2351	3539	6938 -445 1187 - 1724
ANISOU	1520	CC	ASP	220	17.882	31.913	58.502 1.000 42 36
ATOM	1521	001	ASP	220	2653	3531	9912 -812 230 -957
ANISOU	1501	ODI	V C D	420	17.484	31.170	59.423 1.000 37.00
ATOM	1522	ODI	V C D	220	3154	4148	6757 -104 -410 -2001
ANISOU	1522	OD2	VOL.	220	18.981	31.787	57.957 1.000 37.34
ATOM	1523			220	2520	4700	6969 93 -824 -1266
	1523		ALA	221	15.292	30.072	56.537 1.000 24.79
	1524		ALA	221	4148	1872	3398 -252 671 -659
ANISOU	1524		ALA	221	15.695	29.016	55.596 1.000 19.17
ATOM	1525		ALA	221		T898	3251 - 52 - 92 - 610
ANISOU	1525		ALA	221	14.551	27.996	55.479 1.000 18.60
	<b>1 1 2 3</b>	_	ALA	221	1920	2238	2908 -82 -207 - 362
							, == 207 - 302

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			_			- 63 -			
ATOM	1526	0	ALA	221	13.763		56.415	1.000 25	. 47
ANISOU	1526	0	ALA	221	4127	2641	3289	-1307 89	4° - 904
ATOM	1527	CB	ALA	221	16.939	28.316		1.000 19	. 3 6
ANISOU	1527	CB	ALA	221	2054	2333			1666
MOTA	1528		VAL		14.490	27.385	54.313	1.000 17	. 3 5
ANISOU	1528	N	VAL	222	2089	1841	2661	-101 -3	23 - 154
ATOM	1529	CA.	VAL	222	13.556	26.276	54.083	1.000 17	. 4 5
ANISOU	1529	CA	VAL	222	1620	2004	3004	-66 -4	17 1 9
MOTA	1530	С	VAL	222	14.333	24.965	54.077	1.000 15	. 69
ANISOU	1530	С	VAL		1616	1876	2471		49 - 324
ATOM	1531	0	VAL	222	15.512	24.934	53.716	1.000 17	. 8 4
ANISOU	1531	0	VAL	222	1658	1730	3390	-108 -1	9448
ATOM	1532		VAL		12.822	26.433		1.000 19	
UCSINA	1532	CB	VAL		2267	2202	2979	91 -666	- 3 0 4
ATOM	1533				13.781	26.363	51.563		
ANISOU					2252	3113	2977		45 - 182
ATOM	1534				11.730	25.411		1.000 22	
ANISOU					2923	2537	3067		98 4 4
MOTA	1535		LEU		13.789	23.892		1.000 16	
ANISOU			LEU		1792	1694			3 - 5 3 2
MOTA	1536		LEU		14.407	22.575		1.000 15	
UOZINA			LEU		1679	1864	2503		97 – 333
MOTA	1537		LEU		14.114	21.908		1.000 14	
ANISOU			LEU		1337	1537	2773		22 - 458
MOTA	1538		LEU		12.969	21.888		1.000 16	
UOSINA			LEU		1317	2132	2719	70 -391	
MOTA	1539		LEU		13.829	21.779		1.000 19	
ANISOU			LEU		2740	1945	2901		5 -212
ATOM	1540		LEU		14.298	20.348		1.000 23	
ANISOU			LEU		2668	1871	4205		70 9 1
ATOM	1541				15.797	20.322		1.000 23	
ANISOU					2570	3067	3378	69 135 3	
ATOM	1542				13.492 2813	19.668	7459	1.000 35 525 11	116 2333
ANISOU	1542		VAL		15.115	3296 21.370	52.570		
ATOM ANISOU					13.115	1446	2560		320 - 205
ANISOU	1544		VAL VAL		14.956	20.627	51.330		
ANISOU			VAL		1585	1501	2431		323 - 127
ATOM	1545		VAL		15.320	19.160		1.000 1	
ANISOU			VAL		1464	1522	2178	23 -290	-251
ANISOU	1546		VAL		16.442	18.861	51 981	1.000 1	
ANISOU			VAL		1464	1558	2822	0 -505	-374
	1547				15.832			1.000 1	
ANISOU		-			1402	1606	2407		461 - 108
ATOM			. VAL		15.685	20.443		1.000 1	
ANISOU					1682	2164	2474	-159 -	408 - 421
ATOM			VAL		15.575	22.687		1.000 1	
ANISOU					1807	1562	2863	6 -509	
ATOM	1550		PHE		14.340	18.299	51.299	1.000 1	
ANISOU			PHE		1494	1526	2106		353 - 130
ATOM	1551		PHE		14.647	16.882	51.162		4.67
ANISOU			PHE	225		1505	2431	-115 -	61 - 283
ATOM	1552		PHE	225		16.533	49.675	1.000 1	4.27
ANISOU			PHE	225		1533	2352	100 -	260 - 194
ATOM	1553		PHE	225		16.876	48.893	1.000 1	6.25
ANISOU			PHE		1604	2000	2569	296 -	311 - 88
ATOM	1554		PHE	225		15.999	51.749	1.000 1	5.57
ANISOU			PHE	229		1563	2740	-25 -	46 2 4
MOTA	1555	CG	PHE	225	5 13.387	15.996	53.25	7 1.000 1	7.95
ANISOU			PHE		5 1888	2267	2666	-650 -	302 2 0 3
ATOM			1 PHE		5 14.409		54.15	7 1.000 2	7.39





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ATOM	1587	0	ALA	230	18.100	12.091	41.146 1	.000 13.65
ANISOU		-	ALA	230	1240	1530	2418 1	08 4-4 6
MOTA	1588		ALA		16.588	14.000	43 345 1	03 4 4 6 .000 13 66
ANISOU			ALA		1559	1415	2215 -	186 -21 -229
						10.978		.000 13.31
MOTA	1589		THR		17.143	10.978		
ANISOU			THR		1526	1318 9.815 1307		8 -261 - 1
MOTA	1590		THR		18.022	9.815		.000 13.32
ANISOU	1590	CA	THR	231	1660	1307		8 - 302 3 2
MOTA	1591		THR	231	17.906	9.224	41.251 1	.000 13.27
ANISOU			THR		1300	1631		05 -211 3
ANISOU	1592		THR		18.932	8 974		.000 15.51
ANISOU			THR		1468	1631 8.974 1759		45 58 - 170
					17.656	0 751	13 600 1	.000 13.03
ATOM	1593		THR			1202	93.000 I	
ANISOU			THR		1500	8.751 1302 9.313	2151 4	
MOTA	1594				17.530	9.313	44.995 1	.000 14.70
ANISOU	1594	OG1	THR		1742	1614	2230 -	99 32 - 14
MOTA	1595	CG2	THR	231	18.698	7.621 1419 9.049	43.697 1	000 13.69
ANISOU	1595	CG2	THR	231	1449	1419	2335 1	.13 -211 1 9 7
MOTA	1596		LEU	232	16.665	9.049	40.796 1	000 13.43
ANISOU			LEU	232	1447	1384	2271 7	75 -404 - 27
ATOM	1597		LEU		16.446	8.396	39.527 1	.000 14.11
ANISOU			LEU		1809	1384 8.396 1226	2326 8	30 -468 4 9
			LEU		16.975	9.248	28 281 1	1.000 15.53
ATOM	1598		-			1557		209 -3 9 0
ANISOU			LEU		1968	1557 8.808	23/0 2	
$\mathtt{ATOM}$	1599		LEU		17.749	8.808	37.504	1.000 17.16
ANISOU			LEU		2024	1949	2546 1	107 -116 -519
MOTA	1600		LEU		14.940	8.135	39.368	1.000 14.47
ANISOU	1600	CB	LEU	232	1692	1630	2175	72 - 396 - 161
MOTA	1601	CG	LEU	232	14.525	8.135 1630 7.307	38.155	1.000 15.89
ANISOU	1601	CG	LEU	232	1941	1768	2329 :	120 -470 - 303
ATOM			LEU	232	15.118	5.920 2020	38.202	1.000 23.19
ANISOU	1602	CD1	LEU	232	3565	2020	3228	743 -1110 -851
ATOM	1603	CD2	LEU	232	13.003	7.190	38.126	1.000 19.46
ANISOU					2006	2262		-470 -523 - 66
ATOM	1604		VAL		16.539	10.514	38.299	1.000 13.73
ANISOU			VAL		1736		2025	-7 -263 193
ATOM	1605		VAL		16.893	11.317		1.000 13.84
ANISOU			VAL		1674	1658		141 -73 107
			VAL		18.407	11.510		1.000 14.08
ATOM	1606				1716	1674		72 -46 1 1 3
ANISOU			VAL			10/4		1.000 16.65
ATOM	1607		VAL		18.940			38 109 4 0 1
ANISOU					1923	2325	2079	1.000 14.69
MOTA	1608		VAL		16.098			1.000 14.03
ANISOU					1680	1696	2206	141 -165 3 3 3
MOTA			VAL		16.529	13.650		1.000 15.70
ANISOU					1615	1654		34 156 - 28
ATOM	1610	CG2	VAL	233	16.117	13.206	35.647	1.000 16.43
ANISOU	J 1610	CG2	VAL	233	1740	2041	2459	251 117 596
MOTA	1611		THR	234	19.100	11.594	38.175	1.000 14.23
ANISOU			THR		1599	1724	2083	146 -110 2 3 5
ATOM	1612		THR		20.524		38.148	1.000 16.14
ANISOU			THR		1664	1868	2602	63 -171 - 49
ATOM	1613		THR		21.346		38 006	1.000 17.09
					1717	1865	2912	146 211 -51
ANISO			THR				20 120	1.000 17.25
ATOM	1614		THR		4 22.558			108 200 229
ANISO			THR		4 1776	1951	2828	
ATOM	1619				4 21.030			1.000 15.29
ANISO					4 1667	1502	2642	-46 -149 1 6 3
MOTA			1 THR		4 20.849			
ANISO			1 THR		4 1659	1708	2502	-80 59 4 4
MOTA	161	7 CG	2 THR	. 23	4 20.291	13.978	39.597	1.000 16.61
					•			

		PC1/GB98/03860
ANTSON 1617 CCC	- 66 -	
ANISOU 1617 CG2 THE ATOM 1618 N GLV		3077 3 -34 - 12
ANTICOUT ACCOUNT	235 20.712 9 44	3077 3 -34 - 12 1 37.833 1.000 1-5,80
ANISOU 1618 N GLY ATOM 1619 C2 GLY	235 1905 1914	
ANT CON 1 CO	235 21.484 8 20	
ANISOU 1619 CA GLY	235 2049 1861	2506
ATOM 1620 C GLY	235 22.225 7.93	
ANISOU 1620 C GLY	235 2046 2049	
ATOM 1621 O GLY	235 23.285 7.289	
ANISOU 1621 O GLY	235 2167 2606	
ATOM 1622 N GLY	236 21.602 8.149	3303 679 343 <sub>- 74</sub>
ANISOU 1622 N GLY	236 1663 1901	1.000 13.17
ATOM 1623 CA GLY	226 22	
ANISOU 1623 CA GLY		1.000 17.27
ATOM 1624 C GLY	236 23.033 8.639	
ANISOU 1624 C GLY		10.10.88
ATOM 1625 0 GLV	= - 4 4000 109U	2644 204 100 222
ANISOU 1625 O GLY		43.193 1.000 19.42
ATOM 1626 N GIN		
ANISOU 1626 N GLN		41.746 1.000 16.99
ATOM 1627 CA GLN		2957 213 -213 167
ANISOU 1627 CA GLN		
ATOM 1628 C GLM		2752 72 177 9 g
ANISOU 1628 C GLN		4 43.483 1.000 15.64
ATOM 1629 O GLN		2402 231 -146 200
ANISOU 1629 O GLN		2 44.164 1.000 18.17
ATOM 1630 CB GLN		2817 -227 -6 - 4.6
ANISOU 1630 CB GLN		5 41.217 1.000 17.17
ATOM 1631 CG GLN		2532 71 141 - 7
ANISOU 1631 CG GLN		
ATOM 1632 CD GLM		2441 226 95 - 3 n
ANISOU 1632 CD GLM		2 39.137 1.000 19 72
ATOM 1633 OF 1 GIN		2979 104 317 307
ANISOU 1633 OE1 GLN		
ATOM 1634 NE2 CIN		4234 -213 -187 8 0 9
ANISOU 1634 NE2 GLN		1 2 2 3 3 3 3
ATOM 1635 N WAT		2/35 432 374 202
ANISOU 1635 N VAT.		1.000 14.75
ATOM 1636 CA WAT		2237 -32 -54 4 3
ANISOU 1636 CA VAL		
ATOM 1637 C WAT		2388 0 -4432
ANISOU 1637 C VAL		
ATOM 1638 O VAI		2346 82 55 - 1 4 9
ANISOU 1638 O VAL		45.302 1.000 15.87
ATOM 1639 CB VAT.	1039	2737 -218 -285 - 22
ANISOU 1639 CB VAL		44.309 1.000 14.73
ATOM 1640 CG1 VAT		2152 35 -437 - 95
ANISOU 1640 CG1 VAL		45.489 1.000 15.70
ATOM 1641 CG2 WAT		2510 174 -524 - 423
ANISOU 1641 CG2 VAL		43.280 1.000 16 82
ATOM 1642 N TVC		2812 -60 -378 2 2 2
ANISOU 1642 N LYS		47.071 1.000 14.47
ATOM 1643 CA LVS	222 24	2318 14 -40 1 2
ANISOU 1643 CA LVS		48.104 1.000 14 43
ATOM 1644 C IVC		2406 106 -168 1 7 9
ANISOU 1644 C LYS		48.409 1.000 14 82
ATOM 1645 0 1.VS		2642 102 -53 232
ANISOU 1645 O LYS		48.457 1.000 14.74
ATOM 1646 CB LVS	222	2318 158 -275 1 9 0
ANISOU 1646 CB LYS		49.385 1.000 16.40
ATOM 1647 CG LVS		2527 243 -543 252
ANISOU 1647 CG LYS		50.498 1.000 16 65
CO DID	239 1954 1759	2614 -58 -781 2 4 4
		1



ATOM	1648 CD			21.738	9.511	51.683		
ANISOU	1648 CD	LYS	239	2954	1820		-123 :	-1,2,34 363
ATOM	1649 CE	LYS	239	21.107	8.835	52.896	1.000 2	22.58
	1649 CE		239		2164			-1502 863
ATOM	1650 NZ			21.904		54.145		
			239		3360		-471 ·	-943 2 8 7
ANISOU	1650 NZ							
MOTA	1651 N	ALA		18.140	9.892	48.659		
ANISOU		ALA	240		1607			-334 - 61
ATOM	1652 CA	ALA	240	16.791	10.192	49.145		13.98
ANISOU	1652 CA	. ALA	240	1468	1635			-335 - 10
ATOM	1653 C	ALA	240	16.728	9.776	50.605	1.000	13.44
ANISOU		ALA	240		1388		77 -45	
ATOM	1654 0	ALA		16.514	8.592	50.913		
ANISOU		ALA		1932	1567			-673 3 1 4
	1655 CB			15.712	9.565	48.268		
ATOM					1962			
ANISOU	1655 CE			1510		2306		-387 - 307
MOTA	1656 N	PRO		16.907	10.701	51.546		
ANISOU		PRO		1634	1551			-292 7 1
MOTA	1657 CA	PRO		17.035	10.251	52.940		
ANISOU	1657 CA	PRO	241	1718	1681	2180		-174 - 30
ATOM	1658 C	PRO	241	15.693	9.961	53.579	1.000	13.89
ANISOU		PRO	241	1659	1581	2039	-107	-207 - 74
ATOM	1659 0	PRO		14.629	10.527	53.261		
		PRO		1698	1946	2838	17 -25	
MOTA	1660 CE			17.689	11.462	53.619		
	1660 CE			2162	1657		-460	-487 5 5
ANISOU	1661 CC			17.138	12.651			
	1661 CC			2433	1601	2258		-274 3 1
				17.164	12.140			
ATOM	1662 CI				1400	2339	-215	-186 - 66
	1662 CI			1841	1490 9.049 1853	54.544		
ATOM	1663 N	ARG		15.740	3.043	24.244		-308 2 0 4
	1663 N	ARG		1914	1823	2212	-381	
ATOM	1664 C			14.574	8.772	55.376		15.50
	1664 C			1955	1863 9.841	2073	-236	-291 1 8 0
MOTA	1665 C	ARG		14.406	9.841	56.437		
	1665 C	ARG		1889	2011	2407	-120	-411 - 51
ATOM	1666 O	ARG		15.372	10.416	56.994		
ANISOU	1666 O	ARG		2041	2186	2732	-216	-559 - 180
ATOM	1667 C			14.728	7.419	56.085		18.38
ANISOU	1667 C	B ARG	242	2920	1810	2253	-486	-391 2 6 9
ATOM	1668 C	G ARG	242	14.564	6.273 1873	55.094		18.42
ANISOU	1668 C	G ARG	242	2372	1873	2755		162 - 155
MOTA	1669 C	D ARG	242	14.854	4.935	55.796	1.000	23.07
	1669 C		242	3380	2022	3366	470	-483 -217
MOTA	1670 N			16.334	4.954	55.991	1.000	26.69
	1670 N			3498	2727	3916	444	-829 4 7
ATOM	1671 C			16.941	3.921			27.19
ANISOU			242		2879	4284	-297	-1143 802
ATOM	1672 N			16.157	2.913			33.14
	1672 N		242		3235	5546	-316	528 726
ATOM		H2 ARG	242		3.889			31.13
_			242		2925	5859	227	-769 4 8 4
ANISOU		H2 ARG						
ATOM	1674 N		243		10.057			17.55 -173 - 74
ANISOU			243		2233	2457	-165	
MOTA	1675 C		243		11.050			17.84
ANISOU			243		2139	2452	-260	-123 - 75
MOTA	1676 C			11.644	10.627			17.52
ANISO				2102	2084	2470	-248	-164 - 325
ATOM	1677 0							20.23
ANISO				2226	2593	2868	-551	-323 - 392
MOTA	1678 C	B HIS	243	12.865	12.456	57.324	1 1.000	19.74

					- 68 -	
ANISO	U 1678 C			3 2770	2248	2482 -188 -106 8 3
ATOM	1679 C		24	3 11.922	2 12.630	1000
ANISO	U 1679 C	G HIS	24	3 3449	2513	
	1680 N	DI HIS		3 12.209	12.299	2624 164 -382 0 54.879 1.000 25.87
ATOM	U 1680 N	DI HIS	-	3 4780	2575	2.000 23.87
	1681 C	D2 HIS		3 10.633	13.034	56.172 1.000 29.11
ATOM	1682 C	DZ HIS			4490	3348 121 -421 1630
	U 1682 C	el alc		3 11.182		54.109 1.000 32.92
ATOM	1683 N	ES HIC		3 5835	3672	3001 -1102 -1367 600
ANISO	U 1683 N	E2 HTS		3 10.214 3 5719		34.875 1.000 36.95
ATOM	1684 N	HIS		3 3719 4 11.437	4201	4119 1019 -2016 997
ANISO	11	HIS		1 2523	11.194 2477	59.831 1.000 18.87
ATOM	1685 C	HIS		10.302	10.801	2171 -88 -141 -117
ANISO			244	1 2802	2485	3630 174
ATOM	1686 C	HIS	244	9.927	11.968	2628 171 251 272 61.551 1.000 20.33
ATOM	J 1686 C	HIS	244	1803	2969	2052 1.000 20.33
	1687 O J 1687 O	HIS	244	10.482	13.073	2953 -31 -78 -273 61.510 1.000 21.71
ATOM	1688 CE	HIS	244	2057	3418	2774 -535 145 -853
	J 1688 CE	HIS HIS	244	10.714	9.557	61.468 1.000 24 38
ATOM	1689 CG		244	4066	2644	2553 -76 -390 4 4 1
ANISOU	J 1689 CG	HIS	244	11.859 4158	9.725	62.423 1.000 28 34
ATOM	1690 ND	1 HTS	244	13.132	3498	3113 696 -727 - 89
ANISOU	J 1690 ND	1 HIS	244	4012	9.205 <b>447</b> 1	62.268 1.000 32.35
ATOM	רח 1691	2 HIC	244	11.928	10.391	3808 548 -485 -850
ANISOU	1691 CD	2 HIS	244	2937	4137	63.609 1.000 25.21 2505 -373 45 21 9
ATOM	1692 CE	1 HIS	244	13.887	9.531	2505 -373 45 2 1 9 63.312 1.000 31.71
ATOM	1692 CE	1 HIS	244	4157	4277	3613 1224 -749 -518
ANISOU	1693 NE 1693 NE	2 HIS	244	13.146	10.263	64.150 1.000 24.52
ATOM	1694 N	Z HIS VAL	244	3165	3517	2633 94 -82 4 9 2
	1694 N	VAL	245	8.890 2627	11.687	62.349 1.000 23 87
$\mathtt{ATOM}$	1695 CA	VAL	245	8.473	3119	3322 - 251 531 - 310
ANISOU	1695 CA	VAL	245	2785	12.691 3770	63.349 1.000 24.85
ATOM	1696 C	VAL	245	8.624	12.079	2888 481 149 - 293
ANISOU		VAL	245	3220	3558	64.735 1.000 26.03 3112 -289 179 8 9
ATOM	1697 0	VAL	245	8.023	11.025	3112 -289 179 8 9 64.969 1.000 27.98
ANISOU ATOM		VAL	245	3120	3085	4428 42 295 - 5 9
ANISOU	1698 CB 1698 CB	VAL	245	7.020	13.114	63.099 1.000 26.02
ATOM	1699 CG:	VAL	245	2621	3489	3777 94 -103 - 560
ANISOU	1699 CG	I VAL	245	6.586	14.114	64.161 1.000 28.06
111 011	- 1/00 CG2	! VAT.	243	6.927	3330	4614 159 746 -485
ANISOU	1700 CG:	VAL	245	3564	13.705 3809	61.680 1.000 30.51
ATOM	1701 N	ALA	246	9.399	12.696	4220 1264 -305 - 33
ANISOU	1701 N	ALA	246	4338	3787	65.603 1.000 28.08 2543 -850 250 254
ATOM	1702 CA	ALA	246	9.567	12.316	
ANISOU	1702 CA	ALA	246	4363	3360	67.003 1.000 27.45 2707 292 275 3.73
ATOM ANISOU	1703 C	ALA	246	8.356	12.740	2707 292 275 3 7 3 67.833 1.000 32.68
ATOM	1703 C	ALA	246	4915	4473	3031 98 880 1 9 7
ANISOU	1704 0	ALA	246	7.774	13.791	67.563 1.000 29.54
ATOM	1705 CB	ALA ALA	246	3522	4283	3417 -224 875 -329
	1705 CB	ALA	246	10.819 4564	13.010	67.542 1.000 30.33
ATOM	1706 N	ALA	240	8.048	3949	3011 615 -221 - 422
ANISOU	1706 N	ALA	247	4483	11.958	68.849 1.000 34.09
ATOM	1707 CA	ALA	247	7.036	5156 12.190	3311 -1190 466 3 9 3
ANISOU	1707 CA	ALA	247	4188	5627	69.859 1.000 34.23
ATOM	1708 C	ALA	247	7.609	12.910	3189 -1215 315 515
ANISOU	1708 C	ALA	247	5419	4684	71.081 1.000 33.31 2555 249 -506 1147
					-	2555 249 -506 1147



			- 69 -			
ATOM 170	O ALA		12.708	71.523	1.000 3	8.23
ANISOU 170	O ALA	247 5787	4478			1519 1230
	O CB ALA		10.881	70.314	1.000 4	7.11
ANISOU 171	O CB ALA	4 247 8374	6726			464 686
ATOM 171	IN PRO	248 6.817	13.851	71.577		2.28
ANISOU 171		248 5771	5458	4836		33 - 97
ATOM 171	2 CA PRO	248 7.256	14.581		1.000 4	
ANISOU 171		248 7568	5478	3996		413 2 1 4
ATOM 171		248 7.161	13.618	73.948		
ANISOU 171		248 7978	5660	5075	-1446 5	
ATOM 171			12.794	74.014		
ANISOU 171		248 7651	5391	4237		2573 - 796
ATOM 171	5 CB PRO		15.674	72.897		
ANISOU 171	5 CB PRO		4816	5523		L238 - 138
	6 CG PR	0 248 4.973	15.053	72.299		
ANISOU 171		0 248 7228	5564	6545		2210 -1064
	7 CD PR	0 248 5.489	14.272	71.114		
ANISOU 171	7 CD PR	0 248 6395	4579	6006		953 - 577
	8 N AR	G 249 8.109	13.683	74.883	1.000 4	48.76
ANISOU 171	8 N AR	G 249 9141	6341	3045		1069 - 477
	9 CA AR	G 249 7.865	12.783		1.000	55.51
ANISOU 171	9 CA AR	G 249 10023	6914	4156		895 566
ATOM 172	0 C AR	G 249 6.844	13.466		1.000	46.09
ANISOU 172	0 C AR	G 249 5561	8382	3568		-7 1237
	1 0 AR	G 249 6.244	12.915		1.000	56.25
ANISOU 172	1 0 AR	G 249 7572	6368	7433		1799 3995
	2 CB AR		12.459		1.000	55.24
ANISOU 172			7715	4326		2864 1270
	3 CG AR		11.278		1.000	71.04
ANISOU 172			7330	6779		3707 6 2 2
	4 CD AR				1.000	72.89
ANISOU 172			7991	7984		2723 4 0 9
	25 NE AR				1.000	70.73
	25 NE AF		9977	8271		2650 - 266
	26 CZ AF				1.000	12.11
ANISOU 172				7942	2304	2153 1 3 3
	27 NH1 AF				1.000	1622 2074
ANISOU 17			6161	5559	2015	1622 3874
	28 NH2 AF				1.000	0/.00
ANISOU 17			10062		1004	3886 2 2 1
		LA 254 1.981	18.918		1.000	-1437 2347
ANISOU 17		LA 254 15501	7922	8964		
		LA 254 2.287	20.081		1.000	1617 1592
ANISOU 17		LA 254 12510	8110	8286	1.000	60 01
		LA 254 2.943	21.216		-506	2886 1312
ANISOU 17		LA 254 8383	5719	9040		72.37
		LA 254 4.174			1602	4553 3381
ANISOU 17		LA 254 8056	8109	11332	1 1 000	60.48
		LA 254 3.264			-866	4570 - 1112
ANISOU 17		LA 254 12589		3131	- 000 6 1 000	54.40
		LY 255 2.200			594	2922 - 940
ANISOU 17		LY 255 8029	5451	7190		40.05
		LY 255 2.880			1424	836 - 921
ANISOU 17		LY 255 5181	4570	5465	1 1 000	38.82
		LY 255 3.640			557	702 -1561
ANISOU 17		LY 255 4227	4772	5749		39.96
		LY 255 4.580		3 72.39 5715	-128	
		LY 255 2978	6491			37.29
		SER 256 3.164		7 72.50 4527	389	11 - 853
ANISOU 17		SER 256 5047	4594		0 1 000	35.71
ATOM 17	739 CA S	SER 256 3.73	3 20.60	0 /1.42	9 I.UU	

			PCT/GB98/03860
ANTCOU 1222		- 70 -	
ANISOU 1739 CA SE ATOM 1740 C SE ANISOU 1740 C SE ATOM 1741 O SE ANISOU 1741 O SE ATOM 1742 CB SE	ER 256 2.983 ER 256 4584 ER 256 3.251 ER 256 3575	4669 20.000 6107	4019 -98 -85 9 1 69.162 I.000 33.92 3207 503 304 3.72
ANISOU 1742 CB SE ATOM 1743 OG SE ANISOU 1743 OG SE ATOM 1744 N SE ANISOU 1744 N SE ATOM 1745 CA SE	R 256 3125 R 256 2.688 R 256 2987 R 257 2.065 R 257 4037	4830 18.752	71.853 1.000 30.17 3509 624 212 -492 72.601 1.000 61.15 11750 451 1943 263 0
ANISOU 1745 CA SE ATOM 1746 C SEI ANISOU 1746 C SEI ATOM 1747 O SEI ANISOU 1747 O SEI	R 257 2824 R 257 2.378 R 257 3181 R 257 3.359	21.993 5827 22.538 5524 23.159	68.767 1.000 30.95 3109 170 672 -509 67.760 1.000 30.63 2934 -476 765 -1297 68.199 1.000 34.70
ATOM 1748 CB SEF ANISOU 1748 CB SEF ATOM 1749 OG SEF ANISOU 1749 OG SEF ATOM 1750 N ARG	R 257 0.331 R 257 3085 R 257 0.801 R 257 8002 F 258 2.119	6070 23.088 6518 24.361 5175 22.384	69.036 1.000 38.70 5103 796 1381 4 3 5 68.601 1.000 65.12 11565 -999 73375 3 0 2
ATOM 1751 CA ARG ANISOU 1751 CA ARG ATOM 1752 C ARG ANISOU 1752 C ARG ATOM 1753 O ARG	258 2.997 258 3100 258 2.198 258 3488 258 1.132	5068 22.819 4620 22.913 3381 22.294	66.471 1.000 30.51 2855 -332 677 -995 65.396 1.000 28.15 2976 -106 358 -544 64.096 1.000 25.64 2872 -676 273 -904
ATOM 1754 CB ARG ANISOU 1754 CB ARG ATOM 1755 CG ARG ANISOU 1755 CG ARG ATOM 1756 CD ARG	258 3162 258 4.175 258 3158 258 3.861 258 4782 258 5.039	3240 21.873 4041 20.508 3429	63.981 1.000 24.93 3070 -441 478 -560 65.154 1.000 27.21 3141 -446 313 -1352 64.570 1.000 30.90 3531 -737 -738 -389
ANISOU 1756 CD ARG ATOM 1757 NE ARG ANISOU 1757 NE ARG ATOM 1758 CZ ARG ANISOU 1758 CZ ARG ATOM 1759 NH1 ARG	258 5937 258 4.597 258 3372 258 4.633 258 5670 258 5.075	18.176 3858 17.777 2958	64.769 1.000 36.65 4523 106 477 306 64.411 1.000 32.42 5089 -85 -274 5 2 8 63.143 1.000 37.32 5553 155 680 4 3
ANISOU 1759 NH1 ARG ATOM 1760 NH2 ARG ANISOU 1760 NH2 ARG ATOM 1761 N THR ANISOU 1761 N THR ATOM 1762 CA THR	258 3077 258 4.210 258 5812 259 2.806 259 2625	16.566 3151 23.572 3578	62.217 1.000 29.98 4881 -150 -211 -103 62.824 1.000 38.66 5724 -190 -1632 865 63.120 1.000 23.62
ANISOU 1762 CA THR ATOM 1763 C THR ANISOU 1763 C THR ATOM 1764 O THR ANISOU 1764 O THR ATOM 1765 CR	259 2.337 259 2614 259 3.528 259 2257 259 4.698 259 2464	23.482 (2934 23.197 62663 23.411 6	61.730 1.000 21.97 2800 -36 247 -1041 60.808 1.000 19.76 2587 -38 21 -699 51.159 1.000 21.13
ANISOU 1765 CB THR ATOM 1766 OG1 THR ANISOU 1766 OG1 THR ATOM 1767 CG2 THR ANISOU 1767 CG2 THR	259 2297 259 0.760 259 2941	24.793 6 3084 3 25.790 6 2848 3 25.408 6	51.278 1.000 24.04 3927 70 -157 -1229 51.041 1.000 23.14 3648 196 -142 -829 52.331 1.000 25.17
ANISOU 1768 N SER ANISOU 1768 N SER ATOM 1769 CA SER ANISOU 1769 CA SER	260 3.234 260 2386 260 4.225	22.706 5 2762 2 22.515 5	393 726 264 -136 9.600 1.000 20.41 609 -61 74 -806 8.551 1.000 19.33 399 192 8 -344

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ATOM	1770	C	SER	260	3.587	22.871	57 210	1.000 18.78
ANISOU			SER		1996	2544	2595	
								-379 -264 - 311
ATOM	1771	-	SER		2.375	22.758		1.000 21.20
ANISOU	1771		SER	260	1917	2448	3689	-75 -269 - 573
ATOM	1772	CB	SER	260	4.738	21.076	58.480	1.000 20.28
ANISOU	1772	CB	SER		2491	2458	2755	160 -101 - 495
ATOM	1773							
			SER		3.656	20.197		1.000 22.70
ANISOU			SER		2758	2574	3294	-113 -284 -169
ATOM	1774	N	SER	261	4.474	23.329	56.330	1.000 18.79
ANISOU	1774	N	SER	261	2189	2215	2737	-55 -92 3 5
ATOM	1775		SER		4.148	23.585		1.000 16.88
ANISOU								
-			SER		2074	1718	2622	22 -117 -404
ATOM	1776		SER		5.066	22.672	54.106	1.000 17.25
ANISOU	1776	C	SER	261	1720	1833	3000	101 -350 - 491
ATOM	1777	0	SER	261	6.272	22.876		1.000 19.96
ANISOU			SER		1712	2417	3456	50 -483 -781
ATOM	1778		SER					
					4.471	25.028		1.000 19.95
ANISOU			SER		2903	1675	3002	164 -113 - 135
ATOM	1779	OG	SER	261	4.404	25.127	53.107	1.000 35.64
ANISOU	1779	OG	SER	261	5435	4814	3293	-1089 -766 1263
ATOM	1780		VAL		4.467	21.722		1.000 15.56
ANISOU								
			VAL		1751	2021	2140	-75 -40 -436
MOTA	1781		VAL		5.247	20.713	52.711	1.000 15.41
ANISOU	1781	CA	VAL	262	1871	1938	2048	43 21 - 196
ATOM	1782	C	VAL		4.914	20.874		1.000 14.05
ANISOU			VAL		1460	1784	2095	
								-13 29 -144
ATOM	1783		VAL		3.759	20.712		1.000 15.45
ANISOU			VAL		1488	1900	2481	-175 <b>-</b> 94 -191
MOTA	1784	CB	VAL	262	4.902	19.307	53.253	1.000 16.87
ANISOU	1784	CB	VAL		2144	2005	2260	165 -164 2 3
ATOM	1785				5.567	18.275		1.000 20.01
ANISOU					2433	2006	3165	4 -191 -637
MOTA	1786				5.335	19.200	54.715	1.000 18.63
ANISOU	1786	CG2	VAL	262	2390	2242	2446	147 -397 1 7 5
ATOM	1787	N	PHE	263	5.894	21.163		1.000 13.73
ANISOU			PHE		1497	4	2148	5 -64 1 8 6
ATOM								
	1788		PHE		5.762	21.411		1.000 13.04
ANISOU	1788		PHE		1654	1196	2105	-12 -193 1 1 3
ATOM	1789		PHE	263	6.479	20.253	48.284	1.000 13.56
ANISOU	1789	С	PHE	263	1432	1351	2370	-175 -98 -87
ATOM	1790		PHE		7.732	20.177		1.000 13.83
ANISOU	1790		PHE	263	1415			
						1437	2403	-82 -299 -104
ATOM	1791		PHE		6.364	22.770		1.000 13.50
ANISOU	1791	CB	PHE		1658	1374	2098	-295 -97 3 4
ATOM	1792	.CG	PHE	263	6.062	23.148	47.135	1.000 13.34
ANISOU	1792	CG	PHE		1616	1358	2096	-159 -111 8 2
ATOM	1793				6.750	22.635	46.051	
ANISOU					1977	1547	2156	-354 -131 -384
ATOM	1794				5.005	24.048	46.883	1.000 15.37
ANISOU	1794	CD2	PHE	263	1549	1557	2735	-139 -264 3 0 3
ATOM	1795				6.468	22.945	44.720	
ANISOU					1721		2196	
						1621		-242 71 -144
MOTA	1796				4.703	24.366	45.566	
ANISOU					1482	1428	2680	-20 -261 1 3 7
$\mathtt{ATOM}$	1797	CZ	PHE	263	5.383	23.809	44.479	1.000 16.55
ANISOU			PHE		1935	1492	2862	-152 29 1 4
ATOM	1798		PHE		5.721	19.405	47.588	
ANISOU			PHE		1277			66 40 1 0
						1343	1967	-66 -49 1 9
MOTA	1799		PHE		6.267	18.328		1.000 11.90
ANISOU			PHE		1177	1289	2058	-129 34 - 21
MOTA	1800	С	PHE	264	6.440	18.775	45.314	1.000 11.76
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ANISO		PHE	264 1206	1258	2004	-121 -42 8
ATOM	1801 0	PHE	264 5.418	19.097		3 1.000 1.2.55
	1801 0	PHE	264 1165	1473	2133	-77 -120 4 6
ATOM	1802 CB		264 5.346	17.099	46.773	3 1,000 12.39
ANISOU	• •		264 1101	1498		-304 -42 6 3
ATOM	1803 CG		264 5.022	16.558		1.000 13.97
ANISOU	1803 CG		264 1647	1465	2197	-290 13 1 2 1
ATOM	1804 CD	1 PHE	264 5.960	15.848	48.852	1.000 17.07
ANISOU	1804 CD	1 PHE	264 2039	1976		-422 -410 4 9 7
	1805 CD	2 PHE	264 3.747	16.679		1.000 17.41
ATOM	1806 CE	2 PHE	264 1835	2359	2419	-440 433 112
	1806 CE	T PHE	264 5.661	15.247	50.053	1.000 20.59
ATOM	1807 CE	T PHE	264 2616	2710	2496	-556 -425 7 2 5
	1807 CE	2 PHE	264 3.458	16.133	49.906	1.000 22.51
ATOM	1808 CZ	PHE	264 2151 264 4.386	4047	2355	-787 106 553
	1808 CZ	PHE	264 2889	15.350	50.562	1.000 20.88
ATOM	1809 N	LEU	265 7.676	2376		-936 -22 306
ANISOU	1809 N	LEU	265 1192	18.756		1.000 11.81
ATOM	1810 CA	LEU	265 7.900	1248 19.000		
ANISOU	1810 CA	LEU	265 1264	1269		1.000 12.01
ATOM	1811 C	LEU	265 7.915	17.617	2028	-223 16 - 63
ANISOU	1811 C	LEU	265 1266	1298	42.703	1.000 12.10
ATOM	1812 0	LEU	265 8.842	16.834	2033	-117 -81 3
	1812 O	LEU	265 1367	1283	2260	1.000 12.93 -107 -152 4 4
ATOM	1813 CB	LEU	265 9.246	19.730		-107 -152 4 4 1.000 12.59
ANISOU	1813 CB	LEU	265 1399	1364	2019	-257 57 - 9
ATOM	1814 CG	LEU	265 9.500	20.124		1.000 12.19
ATOM	1814 CG	LEU	265 1168	1399	2066	-292 -248 3 0 2
	1815 CD1 1815 CD1	LEU	265 8.620	21.314	41.318	1.000 13.29
ATOM	1816 CD2	LEU	265 1518	1546	1984	84 36 1 9
ANISOU	1816 CD2		265 10.971 265 1204	20.458	41.449	1.000 13.14
ATOM	1817 N	ARG	266 6.842	1593	2197	-234 41 - 20
ANISOU	1817 N	ARG	266 1412	17.249 1127		1.000 12.06
ATOM	1818 CA	ARG	266 6.586	15.913	2043	
ANISOU	1818 CA	ARG	266 1372	1201	2012	1.000 12.07
ATOM	1819 C	ARG	266 6.619	15.965		-258 0 8 0 1.000 11.75
ANISOU		ARG	266 1203	1315	1948	
ATOM	1820 0	ARG	266 6.032	16.860		29 -267 142 1.000 13.06
ANISOU	1820 O	ARG	266 1430	1318	2214	5 -173 281
ATOM	1821 CB	ARG	266 5.243	15.370		1.000 12.95
ATOM	1821 CB	ARG	266 1142	1477	2302	-189 43 - 33
ANISOU	1822 CG 1822 CG	ARG	266 5.036	15.606	43.488	1.000 13.80
ATOM	1823 CD	ARG	266 1351	1686	2207	-159 66 - 115
	1823 CD	ARG	266 3.723	15.041	43.993	1.000 12.70
ATOM	1824 NE	ARG ARG	266 1369	1362	2094	66 -22 8 4
	1824 NE	ARG	266 2.581 266 1343	15.648	43.281	1.000 12.97
ATOM	1825 CZ	ARG	266 1.304	1155	2428	52 -165 -137
ANISOU	1825 CZ	ARG	266 1432	15.281 1009	43.500	1.000 11.34
ATOM	1826 NH1	ARG	266 0.995	14.414	1869	45 -149 -103
ANISOU	1826 NH1	ARG	266 1802	1165	2119	1.000 13.39
ATOM	1827 NH2	ARG	266 0.305	15.821	42.826	-11 -38 7 2
ANISOU	1827 NH2	ARG	266 1490	1067	2210	1.000 12.55 125 -357 - 159
ATOM	1828 N	PRO	267 7.237	14.951	39.357	
ANISOU	1828 N	PRO	267 1418	1394	2030	16 -146 108
ATOM	1829 CA	PRO	267 7.298	14.947	37.887	1.000 13.88
ANISOU	1829 CA	PRO	267 1442	1786	2047	167 -125 - 8 4
	1830 C 1830 C	PRO	267 5.957	14.722	37.222	1.000 12.61
	1030 (	PRO	267 1413	1508	1868	-6 44 2 7

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ATOM	1831	0	PRO	267	4.998	14.155	37 772	1 000	13.60
ANISOU	1831		PRO	267	1648	1355	2164		
ATOM	1832		PRO	267		13.761		-160	
	1832		PRO	267	1435	1740	37.599		15.30
ATOM	1833		PRO	267			2637	115	-28 -169
	1833		_			12.846	38.764		
			PRO	267	1885	1804	2324	381	-270 -197
ATOM	1834		PRO	267	7.872	13.746	39.965	1.000	14.73
	1834		PRO	267	1803	1356	2438	311	-666 - 205
ATOM	1835		ASN	268	5.933	15.051	35.939	1.000	13.27
ANISOU			ASN	268	1601	1665	1777	-126	-43 -127
$\mathtt{ATOM}$	1836		ASN	268	4.800	14.709	35.073		13.72
ANISOU	1836	CA	ASN		1793	1401	2018	-214	-236 - 71
ATOM	1837	C	ASN		4.723	13.192	34.875	1 000	12 14
ANISOU	1837	С	ASN		1485	1350	2156		
ATOM	1838		ASN		5.702	12.467		-213	104 5 4
ANISOU	1838		ASN		1698	1416	34.934		13.90
ATOM	1839		ASN				2167	-91	123 - 36
ANISOU				268	4.997	15.338	33.690		15.74
			ASN		2597	1369	2016	-66	-437 1 3 5
ATOM	1840		ASN		5.011	16.862	33.811		15.41
ANISOU	1840		ASN		2255	1439	2162	-17	-184 4 7
MOTA	1841	OD1	ASN		4.069	17.454	34.352	1.000	17.75
ANISOU	1841	OD1	ASN		2573	1686	2487	42 91	
ATOM	1842	ND2	ASN	268	6.066	17.503	33.319		16.61
ANISOU	1842	ND2	ASN	268		1355	2546	-50	-57 142
ATOM	1843		ALA		3.531	12.712	34.594		13.99
ANISOU			ALA		1677	1467	2172		
ATOM	1844		ALA		3.278	11.286		-356	-65 170
ANISOU			ALA		1459		34.353		13.42
ATOM	1845					1405	2234	-208	-118 1 0 7
ANISOU			ALA	269	4.182	10.729	33.252		13.93
			ALA		1289	1538	2466	-168	-5 1 5 3
ATOM	1846		ALA		4.581	9.550	33.318		14.97
ANISOU			ALA	269		1476	2494	-143 <sup>-</sup>	112 8 6
MOTA	1847		ALA		1.806	11.051	34.008		13.76
ANISOU	1847		ALA	269	1300	1474	2454	-60	-61 123
$\mathtt{ATOM}$	1848		ASP	270	4.482	11.541	32.251		14.38
ANISOU	1848	N	ASP		1688	1476	2300	-151	30 - 5
ATOM	1849	CA	ASP		5.247	11.079	31.098		
ANISOU	1849		ASP		1747	1693	2194	-99	
ATOM	1850		ASP		6.749	11.287			
	1850		ASP		1714		31.227		15.68
MOTA	1851		ASP		7.483	1886	2357	-224	143 8 6
ANISOU	1851					11.008	30.255	1.000	
			ASP		1952	2354	2200	-80	139 226
ATOM	1852	CB	ASP		4.718	11.681	29.800		17.67
ANISOU			ASP		2461	1966	2288	-75	-319 1 2 6
MOTA	1853		ASP		4.968	13.168	29.649	1.000	18.22
ANISOU	1853		ASP	270	2284	2024	2613	-88	-80 474
$\mathtt{ATOM}$	1854	OD1	ASP	270	5.386	13.826	30.607		
ANISOU	1854	OD1	ASP		3424	1541	2844	-47	-287 4 2 5
ATOM	1855				4.646	13.698	28.552		
ANISOU	1855				3317	2727	2719		
ATOM	1856		PHE		7.221			-49	-136 8 1 2
ANISOU	1856	NI				11.668			13.93
ATOM			PHE		1556	1318	2417	97 31	
	1857		PHE		8.671	11.723			14.41
ANISOU	1857		PHE		1624	1430	2423	110	29 2 6 3
ATOM	1858		PHE	271	9.275	10.349	32.325	1.000	13.31
ANISOU			PHE		1402	1430	2225	-30	28 2 1 8
MOTA	1859		PHE	271	8.790	9.340			14.91
ANISOU	1859	0	PHE		1900	1374	2392	-26	240 192
MOTA	1860		PHE		8.942	12.146	34.098		15.57
	1860		PHE		1700	1721	2495		
ATOM	1861		PHE		10.386			-66	-36 9
	1001		THE	211	10.300	11.791	34.516	1.000	14.56

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ANISOU			PHE	271	1729	1320	2485	-152 34 -124
ATOM	1862	CD1	PHE		11.460	12.369		1.000 1~7~. 76
ANISOU	1862	CD1	PHE	271	1714	1581	3452	
ATOM	1863	CD2	PHE		10.698	10.972		-235 393 -249 1.000 18.04
ANISOU		CD2	PHE		2182	1543	3130	
ATOM	1864				12.786	12.092		-95 -540 1 7 2
ANISOU		CE1	PHE	271	1838	1700	34.166	1.000 17.54
ATOM	1865	CE2	PHE	271	11.997		3128	-291 114 -50
ANISOU	1865	CE2	PHF	271	1935	10.609 1646	35.899	
ATOM	1866	C 7:	PHE		13.039	11.154	3578	-392 -396 4 2 5
ANISOU	1866		PHE	271	2444	1697	35.162	
ATOM	1867		THR	272	10.278	10.298	2415	-486 -19 -394
ANISOU	1867		THR	272	1514	1641	31.453	1.000 13.78
ATOM	1868	CA	THR		10.811	9.046	2083	30 19 1 5 4
ANISOU	1868		THR	272	1551	1660	30.938	1.000 13.99
ATOM	1869		THR	272	12.246	8.841	2105	-99 83 6 7
ANISOU	1869		THR	272	1598	1549	31.410	
ATOM	1870		THR		13.046	9.808	2441	-3 108 3 5 7
ANISOU	1870		THR		1646	1742	31.424	1.000 16.23
ATOM	1871		THR		10.751	9.117	2780	-246 5 185
ANISOU			THR	272	1856	2205	29.388	1.000 16.27
ATOM	1872		THR	272	9.341	9.221	2119	191 125 8
ANISOU	1872	OG1	THR	272	1996	2473	29.032	
ATOM	1873	CG2	THR	272	11.249	7.856	2368	64 -190 264
ANISOU	1873	CG2	THR	272	2423	2167	28.723	1.000 17.94
ATOM	1874	N	PHE	273	12.567	7.600	2227	173 177 - 94
ANISOU	1874		PHE	273	1644	1521	31.743	
ATOM	1875	CA	PHE		13.894	7.253	2499	92 238 2 1 8
ANISOU		CA	PHE	273	1602	1813	32.254	1.000 15.16
ATOM	1876	C	PHE	273	14.350	5.899	2345	296 277 5 5
ANISOU			PHE	273	1408	1647	31.724	1.000 14.69
ATOM	1877		PHE		13.541	5.086	2528	24 479 1 7 8
ANISOU	1877		PHE	273	1738	1767	31.262	1.000 15.91
ATOM	1878		PHE	273	13.899	7.301	2541	-115 450 119
ANISOU			PHE	273	1758	1921	33./69	1.000 15.77
ATOM	1879		PHE		12.931	6.336	2314	-344 286 123
ANISOU	1879		PHE	273	1390	1726	34.424	1.000 14.54
ATOM	1880			273	11.601	6.743	2410	-95 -11 195
ANISOU				273	1457	2343	34.655	<del>-</del> -
ATOM	1881	CD2	PHE	273	13.295	5.038	2521	-24 308 362
ANISOU	1881	CD2	PHE	273	1863	1624	34./21	1.000 15.23
ATOM	1882	CE1	PHE	273		5.848	2300	-110 91 136
ANISOU	1882	CE1	PHE		1593	2158	33.239	1.000 16.10
ATOM	1883	CE2	PHE		12.419	4.148	2365	-162 292 122
ANISOU	1883	CE2	PHE	273	1904	1980	33.354	1.000 16.01
MOTA	1884	CZ	PHE	273	11.109	4.559	2198	-139 285 181
ANISOU			PHE	273	1843	2001	1005	1.000 15.18
ATOM	1885		SER	274	15.634	5.612	1925	-141 73 -227
ANISOU			SER	274	1559	1940	31.926	1.000 15.31
ATOM	1886		SER		16.221	4.318	2317	361 383 247
ANISOU	1886	CA	SER		1476	1723	2642	1.000 15.37
ATOM	1887		SER		15.953	3.284		32 557 1 5 6
ANISOU	1887		SER	274	973 187	3.284 7 272	J2.588	1.000 14.67
MOTA	1888		SER	274	16.310	3.476	26 -11	13 265 3 0 2
ANISOU	1888		SER	274	1668	1677	2728	1.000 15.98
ATOM	1889		SER		17.742	4.556		126 143 193
ANISOU	1889		SER		1487	2019	31.356	1.000 17.41
ATOM	1890		SER		18.362	3.280	3112	235 945 725
ANISOU	1890	ŌĞ	SER	274	1839	1961	31.334	1.000 18.03
ATOM	1891		VAL	275	15.395	2.133	3052	293 840 188
	1891		VAL	275	1646	1857	32.182	
				-, -	-0-0	1001	2417	-182 461 261

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MOTA	1892		VAL	275 15.158	1.033	33.137	1.000 15.65
ANISOU			VAL	275 1681	1800	2466	-180 2 <b>61</b> ,265
ATOM	1893		VAL	275 16.454		33.659	1.000 15.33
ANISOU			VAL	275 1805	1881	2139	116 392 - 45
ATOM ANISOU	1894		VAL	275 16.623	0.280		1.000 15.68
ANISOU	1895		VAL VAL	275 2037 275 14.227	1655	2267	6 297 1 9 6
ANISOU			VAL	275 14.227	-0.004 1708	2755	1.000 16.05
ATOM	1896			275 14.080	-1.186		-76 405 2 1 1.000 17.04
ANISOU				275 2045	1688	2740	-211 230 1 5
MOTA	1897			275 12.847	0.608		1.000 18.45
ANISOU				275 1650	2432	2928	-57 135 269
ATOM	1898		PRO	276 17.437			1.000 16.21
ANISOU			PRO	276 1927	1700	2532	97 589 3 6
ATOM ANISOU	1899 1899		PRO PRO	276 18.707	-0.434		1.000 18.10
ANISOU	1900		PRO	276 1736 276 19.382	2115 0.541	3025	147 616 - 93
ANISOU			PRO	276 19.382	1961	2697	1.000 17.52 97 469 2 3 9
ATOM	1901		PRO	276 19.963	1961 0.171		1.000 19.66
ANISOU	1901	0	PRO	276 2015	2409	3047	24 280 4 6 8
MOTA	1902		PRO	276 19.590			1.000 20.80
ANISOU			PRO	276 2094	2687	3121	306 771 - 249
ATOM	1903		PRO	276 18.852	-0.390		1.000 21.57
ANISOU ATOM	1903		PRO PRO	276 2051 276 17.446	3098	3046	340 802 - 288
ANISOU			PRO	276 2053	-0.021 2306	2546	1.000 18.17 179 832 - 318
ATOM	1905		LEU	277 19.325	1.845		179 832 - 318 1.000 17.09
ANISOU	1905	N	LEU	277 1571	1898	3025	230 511 1 0 7
MOTA	1906		LEU	277 19.962	2.802		1.000 19.34
ANISOU			LEU	277 2035	2141	3171	-219 218 262
ATOM ANISOU	1907		LEU LEU	277 19.214	2.858		1.000 18.34
ATOM	1907		LEU	277 1963 277 19.815	1958 2.957	3049	-33 -3 - 3 8 1.000 19.29
ANISOU			LEU	277 2466	1710	3154	-271 -188 - 2
MOTA	1909	СВ	LEU	277 20.094	4.178		1.000 21.41
UOSINA			LEU	277 2739	2011.	3383	14 12 2 8 7
ATOM	1910		LEU	277 20.910	5.192		1.000 26.34
ANISOU ATOM			LEU	277 3662	2367		-980 -547 9 4 4
ANISOU	1911	CDI	PEO	277 22.396 277 3764	4.839		1.000 38.04
ATOM	1912			277 20.708	3171 6.607	7518	-487 -2057 853 1.000 31.98
ANISOU				277 4023	2018		
ATOM	1913	N	ALA	278 17.875	2.711	36.202	1.000 17.30
ANISOU			ALA	278 2015	1766	2793	74 218 1 1 5
ATOM	1914		ALA	278 17.124	2.712		1.000 16.75
ANISOU ATOM	1914		ALA ALA	278 2200	1566	2600	216 146 - 2
ANISOU			ALA	278 17.575 278 1849	1.523 1553	38.313 2794	1.000 16.31 -337 -196 1 0 7
ATOM	1916		ALA	278 17.718	1.635		-337 -196 1 0 7 1.000 1 7 . 2 6
ANISOU			ALA	278 1963	1839	2754	-62 -53 2 0 5
ATOM	1917		ALA	278 15.642	2.622		1.000 17.55
ANISOU			ALA	278 2109	1880	2679	295 195 - 11
ATOM	1918		ARG	279 17.724			1.000 17.07
ANISOU ATOM	1918		ARG ARG	279 2322 279 18.099	1399	2766	-178 26 3 0 8
ANISOU			ARG	279 18.099	-0.829 1734	38.473 2323	1.000 16.93 15 -241 203
ATOM	1920		ARG	279 19.477	-0.587		15 -241 203 1.000 19.87
ANISOU	1920	С	ARG	279 2491	2292	2766	-487 -384 5 4 3
ATOM	1921		ARG	279 19.687	-0.974		1.000 33.04
ANISOU			ARG	279 3615	4823	4115	-1726 -1700 2603
ATOM	1922	CB	ARG	279 18.164	-2.042	37.517	1.000 20.04
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	1922		ARG	279	2042	1609	3964	108	-221 - 305
ATOM	1923	CG	ARG		16.742	-2.491	37.179	1 000	) 2-0-,73
ANISOU			ARG		2152	2728	2997	-98	-401 - 351
ATOM	1924		ARG		16.601	-3.422		1:000	24.81
ANISOU ATOM			ARG		3213	2982	3231	-1 -5	07 - 609
	1925 ; 1925 ;	NE	ARG	279	17.575	-4.484	36.195	1.000	27.50
ATOM	1926		ARG	279	4331	2656	3463	355	-146 - 181
	1926	C 2	ARG	2/9	17.301	-5.725	36.620	1.000	41.33
ATOM	1927	C Zi	ARG	2/9	7720	2466	5519	-186	-454 - 142
ANTSOU	1927	NH 1	ARG	2/9	16.024	-6.012	36.866	1.000	40.58
ATOM	1928	MHO	ARG	2/9	8821 18.200	3012	3585	-1564	507 452
	1928	NH2	ARG	279	9516	-6.688	36.807	1.000	53.27
MOTA	1929 1		GLU	280	20.390	2227	8496	-127	-4607 -463
	1929 1		GLU	280	2172	0.119 2276	38.424	1.000	19.68
ATOM	1930 (	CA	GLU	280	21.748	0.334	3028	84 32	4 1 3 6
ANISOU	1930 (		GLU	280	2046	2274	38.948	1.000	20.28
ATOM	1931 (	2	GLU		21.705	1.257	3385	25 58	1 1 1 5
ANISOU	1931 (		GLU	280	2334	1968	40.182 3552		
$\mathtt{ATOM}$	1932 (	C	GLU		22.723	1.079	40.908	-281	285 2 0
ANISOU	1932 (	)	GLU		2659	3419	4107	-37	
ATOM	1933 (		GLU		22.651	1.029	37.926	1 000	-183 - 87
ANISOU			GLU	280	2778	2558	4044	-351	1022 3 0 3
ATOM	1934 (		GLU	280	22.997	0.342	36.634	1 000	27 13
ANISOU			GLU		2605	4888	2816	596	116 623
ATOM	1935		GLU	280	23.815	1.298	35.760	1.000	43 10
ANISOU ATOM			GLU		4693	7780	3903	-1328	1206 8 3 4
AIUM	1936	DEL	GLU	280	24.541	2.171	36.296	1.000	41.36
ANISOU ATOM	1936 (	DET (	GLU	280	2666	6033	7015	27 10	99 690
ANISOU	1937	DEZ (	GLU	280	23.727	1.219	34.520	1.000	64.81
ATOM	1938 N				10844	10028	3751	-2356	1104 2134
ANISOU	1938 N		CYS CYS	281	20.777	2.156	40.313	1.000	21.61
ATOM	1939 C		CYS		2372	2240	3599	-211	532 - 238
ANISOU	1939		CYS		20.481 2114	3.164	41.337	1.000	
ATOM	1940 C		CYS	201	19.858	2911	4219	-526	1121 - 817
ANISOU			CYS	201	2492	2.568	42.585	1.000	27.11
ATOM	1941 C		CYS		19.789	3261 3.161	4546	-1608	1457 - 1343
ANISOU	1941 C		CYS	281	1997	2012	43.685	1.000	19.19
ATOM	1942 C		CYS	281	19.632	4.438	3282	-250	-326 1 3 5
ANISOU	1942 C		CYS	281	1214	3088	40.795		
ATOM	1943 S	G (	CYS	281	20.639	5.092	4063	-286	100 -2108
ANISOU		G (	CYS	281	10822	4742	39.444 4730	1.000	53.41
ATOM	1944 N	1 (	GLY		19.370	1.317	42.565	1- 000	1316 4 5
ANISOU			GLY		1230	2224			18.81 19 -206
ATOM	1945 C	:A (	${ t GLY}$		18.675	0.750	43.744		17 - 200 17 - 07
ANISOU			GLY	282	1544	1771	3171	31 -5	52 - 168
ATOM	1946 C		GLY	282	17.194	0.496	43.538	1 000	1 / 01
ANISOU	1946 C		GLY	282	1601	1645	2417	-135	-453 3 7 8
ATOM	1947 0		GLY	282	16.480	-0.062	44.380	1.000	16 38
ANISOU			GLY	282	1998	1921	2306	-211	-399 3 6 0
ATOM	1948 N		PHE	283	16.625	0.919	42.404	1.000	13.44
ANISOU ATOM	1948 N		PHE	283	1563	1539	2006	-189	-336 -115
ANISOU	1949 0		PHE	283	15.173	0.829	42.203	1.000	14.52
ATOM	1949 C		PHE	283	1677	1410	2428	-187	-670 4 6
ANISOU	1950 0		PHE	283 203	14.810	-0.604	41.809	1.000	13.08
ATOM	1951 0		PHE	∠ Ø 3	1519	1314	2137	-121	-338 1 7 4
ANISOU	1951 0		PHE PHE	203	15.311	-1.184	40.837		14.11
ATOM	1952 C		PHE	203	1366	1418	2578	-142	-78 1 7
ANISOU	1952 C		PHE	203	14.749	1.800	41.078	1.000	
		1 ك	LIIC	203	1814	1288	2125	-39	-268 0

ANISOU 1980 N

ANISOU 1982 C

ANISOU 1981 CA LEU

1982 C

1983 0

ATOM

ATOM

MOTA

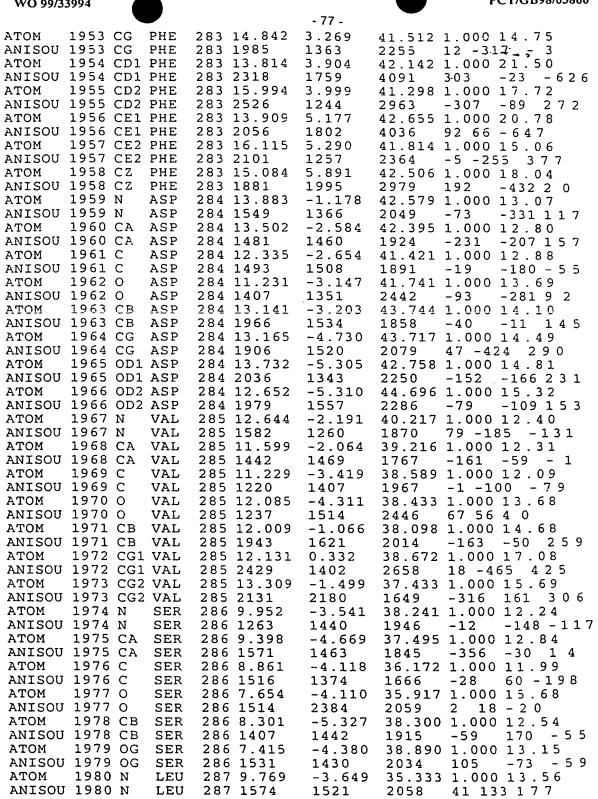
LEU

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1981 CA LEU



287 1945

287 1574 1521 2058 41 133 1 7 7 287 9.451 -2.932 34.101 1.000 13.48 287 1812 1418 1891 -84 116 1

287 10.075 -3.654 32.908 1.000 15.12

287 11.277 -3.883 32.927 1.000 17.91

1714

2086

1891 -84 116 1 7

32 233 - 31

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ANISO ATOM	0 198	3 0	LEU	28	7 1885	2275	2645	109	300 - 275
ANISO	198	4 CB	–	28	7 9.954	-1.480			0.1.4 <u>.</u> .37
ATOM	100	4 CB 5 CG		28.	7 1773	1380	2306	-34	248 107
ANISO	190. 199: Ti	5 CG		28	7 9.362	-0.603	35.231	1:000	0 14.32
ATOM	198	2 CG	LEU 1 LEU	287		1496	2523	62 52	2 - 158
ANISO	198	S CD	1 LEU	287		0.705	35.413	1.000	14.53
ATOM		7 CD	2 LEU	287	7 1672 7 7.921	1444	2403	0 -1	146 143
ANISOU	J 198	7 CD	2 LEU	287	7 1476	-0.197		1.000	16.03
$\mathtt{ATOM}$	1988	3 N	ASP		9.256	2035 -4.060		166	-100 - 7
JOSIKA			ASP	288	3 2041	1611	31.958		15.09
ATOM	1989	CA	ASP	288	9.764	-4.722	2081		75 - 216
ANISOU	J 1989	CA	ASP	288	1992	2028	2268	1.000	16.55
ATOM ANISOU	1990	C	ASP	288	10.437	-3.682	29.874	1 000	35 - 314 ) 18.74
ATOM	1990		ASP	288	2484	2597	2040	-231	97 8 1
ANISOU	נפפג 1991 ז	. 0	ASP	288	9.998	-2.526	29.849	1.000	25.48
ATOM	1992	CR	ASP ASP	288	3382	2433	3865	-322	639 346
ANISOU	1992	CB	ASP	200	8.659 2431	-5.490	30.060	1.000	19.23
ATOM	1993	CG	ASP	288	9.139	2414	2460	-209	258 - 720
ANISOU	1993	CG	ASP	288	2688	-6.468 2223	29.000	1.000	19.50
ATOM	1994	OD1	ASP	288	10.173	-7.145	2499	-49	393 - 552
ANISOU	1994	OD1	ASP	288	3134	3038	4100	1.000	27.03
ATOM	1995	OD2	ASP	288	8.458	-6.566		624	427 - 716 31.00
ANISOU ATOM	1995	OD2		288	3596	4859		307	-361 -2100
ANISOU	1996	N	GLY	289	11.489		29.137	1.000	22.68
ATOM	1997	C 2	$\mathtt{GLY}$	289	2960	2893	2765	-531	778 116
ANISOU	1997	CA	GLY	289	12.008 3678	-3.083	28.169	1.000	25.60
ATOM	1998	С	GLY	289	12.988	3562	2486	-1469	558 1 1
ANISOU	1998	С	GLY	289	2567	-2.078 2916	28.725	1.000	21.08
ATOM	1999	0	$\mathtt{GLY}$	289	13.411	-2.097	2528	-485	353 150
ANISOU			GLY	289	3428	3219	29.891 2364	-1104	43.72
ATOM ANISOU	2000	N	GLU	290	13.402	-1.168	27.818	1.000	440 113
ATOM	2001	LN N	GLU	290	2246	2396	2319	-145	616 -115
ANISOU	2001	CA	GLU GLU	290	14.538 1912	-0.301	28.074	1.000	17.75
ATOM	2002	C	GLU	290	1912	2419	2412	97 77	0 - 367
ANISOU	2002	Ċ	GLU	290	2180	1.058	28.696	1.000	17.90
MOTA	2003	0	GLU	290	15.143	2308 1.619	2313	50 71:	1 - 2 9 7
ANISOU			GLU	290	2525	2050	29.353 2104	-35	17.58
ATOM	2004		GLU	290	15.341	-0.161		1 000	380 165 23.21
ANISOU ATOM	2004	CB	GLU	290	3184	2508	3126	-273	1753 - 467
ANISOU	2005	CG	GLU	290	15.833	-1.492	26.226	1.000	24.55
ATOM	2006	CD	GLU	290	3609	2992	2725	348	1232 - 743
ANISOU	2006	CD	GLU GLU	290	16.676	-2.280	27.221	1.000	30.03
MOTA	2007	OE1	GLU	290	3365 17.492	3708	4337	476	753 - 211
ANISOU	2007	OE1	GLU	290	5043	-1.684 6674	27.947	1.000	
ATOM	2008	OE2	GLII	290	16.622	-3.527	3498	525	36 -1226
ANISOU	2008	OE2	GLU	290	8785	3812	27.237 7070	1.000	
ATOM	2009	N	THR	291	13.064	1.578	28.486	-12 1 000	-483 1583
ANISOU ATOM	2009	_	THR	291	2305	2486	2103	224	711 - 321
ANISOU	2010		THR	291	12.697	2.896	29.049	1.000	18.72
ATOM	2011		THR THR	291	2521	2080	2511	105	1131 6 6
ANISOU	2011		THR	231 201	11.278 2178	2.744	29.593	1.000	15.79
ATOM	2012	0	THR	291	10.517	1758	2064	134	538 - 50
ANISOU	2012	0	THR	291	2764	1.834 1966			18.62
ATOM	2013	CB	THR		12.722	4.031	2344	-248	664 - 311
ANISOU	2013	CB	THR	291	3043	2625	28.044 2516	-164	
								T 0 4	891 362

						73-		
MOTA	2014	0G1	THR	291	11.695	3.862	27 077	1.000 25.98
ANISOU					3160	4072	2641	-86 <b>7</b> 03 5 0 3
ATOM	2015							
					14.048	4.115		1.000 24.20
ANISOU					3199	3832	2164	-445 930 533
ATOM	2016	N	ALA	292	10.959	3.658	30.492	1.000 14.84
ANISOU	2016	N	ALA		1637	1656	2347	200 429 -153
ATOM	2017		ALA		9.675			
						3.657	31.179	1.000 13.84
ANISOU			ALA		1488	1477	2294	170 299 7 8
ATOM	2018	C	ALA	292	9.356	5.065	31.619	1.000 12.65
ANISOU	2018	С	ALA	292	1334	1564	1908	60 144 - 139
ATOM	2019		ALA		10.228	5.939	31.710	
	2019		ALA	202	1529			
						1596	2295	-35 109 116
MOTA	2020		ALA		9.670	2.754	32.414	1.000 14.02
ANISOU	2020	CB	ALA	292	1693	1580	2053	37 22 - 27
ATOM	2021	N	THR	293	8.054	5.258	31.916	1.000 13.54
ANISOU	2021	N	THR		1468	1617	2058	117 373 - 118
ATOM	2022		THR		7.605	6.546		
								1.000 13.40
ANISOU			THR		1565	1647	1877	152 209 - 232
MOTA	2023		THR		7.407	6.482	33.952	1.000 12.09
ANISOU	2023	С	THR	293	1345	1322	1927	-62 326 -12
ATOM	2024		THR		7.214	5.441	34.555	
ANISOU			THR		1385	1356		
							2170	-190 194 9 0
ATOM	2025		THR		6.295	7.058		1.000 13.45
ANISOU			THR		1598	1579	1935	95 345 3 4 5
ATOM	2026	OG1	THR	293	5.273	6.112	32.117	1.000 13.75
ANISOU	2026	OG1	THR		1672	1570	1981	-12 314 135
ATOM	2027				6.476	7.139	30.272	
ANISOU								
					2121	2022	1911	255 434 337
ATOM	2028		PHE		7.241	7.661		1.000 12.81
ANISOU	2028	N	PHE		1607	1440	1822	-83 149 -151
ATOM	2029	CA	PHE	294	6.857	7.773	35.935	
ANISOU	2029	CA	PHE		1332	1469	1899	-267 166 -289
ATOM	2030		PHE		5.556	7.022		1.000 12.36
ANISOU								
			PHE		1336	1361	1999	-151 30 - 36
ATOM	2031		PHE		5.403	6.253	37.143	1.000 13.27
ANISOU	2031	0	PHE	294	1556	1410	2076	-191 183 4 6
ATOM	2032	CB	PHE	294	6.698	9.271	36,267	1.000 13.83
ANISOU	2032	CB	PHE	294	2039	1351	1866	-192 -29 -177
ATOM	2033		PHE		6.306	9.488		1.000 13.10
ANISOU								
			PHE	294		1216	1974	-125 -63 -244
ATOM	2034	CDI	PHE		7.207	9.411		1.000 17.41
UOSINA				294	2132	2533	1952	-1012 -287 7 6
MOTA	2035	CD2	PHE	294	4.964	9.739	38.026	1.000 18.41
ANISOU	2035	CD2	PHE	294	2156	2263	2575	565 332 5 7
ATOM	2036				6.810	9.608		1.000 17.72
ANISOU	2036	CEI	DILL					
					2348	2296	2086	-308 -362 -136
MOTA	2037				4.591	10.010	39.324	1.000 19.37
ANISOU	2037	CE2	PHE	294	2078	2541	2740	330 232 -630
ATOM	2038	CZ	PHE	294	5.507	9.956	40.355	
ANISOU			PHE		2443	1678	2855	-394 -55 -245
ATOM	2039						2033	
			GLN		4.588	7.205		1.000 12.59
ANISOU			GLN	295	1248	1429	2106	-62 38 - 168
ATOM	2040		GLN	295	3.320	6.484	35.408	1.000 12.76
ANISOU	2040	CA	GLN	295	1266	1215	2365	7 -157 -117
ATOM	2041		GLN		3.512	4.984	35 310	1.000 12.24
ANISOU			GLN	295				
						1256	1944	10 1 - 7 3
ATOM	2042		GLN	295		4.238		1.000 13.61
ANISOU			GLN	295		1427	2424	7 85 1 5 5
ATOM	2043	CB	${\tt GLN}$	295	2.375	6.975	34.317	1.000 14.31
ANISOU	2043	СВ	GLN	295	1227	1594	2616	81 -133 192
ATOM	2044	CG	GLN		1.062	6.256		1.000 14.03
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ANISO			GLN	295 1391	1509	2430	-59 -300 4 7
ATOM	2045	5 CD	GLN	295 0.157	5.687	5420	-59 -300 4 7 5 1.000 13 56
ANISO	J 2045	CD	GLN	295 1305	1486	2361	
ATOM	2046	0E	GLN	295 0.459	7.693	2301	133 -117 1 6 5
ANISOU	J 2046	OE:	LGLN	295 1811	1651	32.415	1.000 15.35
$\mathtt{ATOM}$	2047	NE2	2 GLN	295 -0.982	6.026	2371	161 206 220
ANISOU	2047	NE2	GLN	295 1225		32.943	
ATOM	2048	N	ASP	296 4.363	1995	2493	
ANISOU	1 2048	N	ASP	296 1425	4.463	34.423	1.000 12.66
ATOM	2049		ASP	296 4 652	1396	1990	181 -112 - 110
ANISOU	2049	) CA	ASP	296 4.653	3.016	34.439	1.000 12.26
ATOM	2050		ASP	296 1628	1274	1755	53 -51 -151
ANISOU	2050		ASP	296 5.167	2.569	35.792	1.000 11.57
ATOM	2051		ASP	296 1199	1300	1895	-82 30 - 22
ANISOU	2051	. 0		296 4.854	1.460	36.224	1.000 13.08
ATOM	2051		ASP	296 1534	1368	2070	-107 38 1 3 9
ANISOU			ASP	296 5.709	2.634	33.399	1.000 14.18
ATOM			ASP	296 1870	1700	1819	141 30 - 378
	2053	CG	ASP	296 5.295	2.848	31.952	1.000 13.32
ANISOU			ASP	296 1655	1557	1848	-58 67 2
ATOM	2054	OD1	ASP	296 4.110	2.725	31.601	1.000 15.83
ANISOU	2054	OD1	ASP	296 1680	1935	2402	-68 -126 - 189
ATOM	2055	OD2	ASP	296 6.212	3.098		1.000 15.27
ANISOU	2055	OD2		296 1757	1937	2106	-229 137 177
ATOM	2056	N	TRP	297 6.038	3.352		-229 137 177 1.000 12.26
ANISOU	2056	N	TRP	297 1325	1403	1931	
ATOM	2057	CA	TRP	297 6.683	2.960		
ANISOU			TRP	297 1328	1599	3/.030	1.000 12.82
ATOM	2058	С	TRP	297 5.746	3.007	1943	-104 -49 151
ANISOU	2058	С	TRP	297 1418	1580	38.858	1.000 13.13
ATOM	2059	0	TRP	297 5.565	2.030	1992	24 -23 1 8 5
ANISOU	2059	O	TRP	297 1554	1619	39.584	1.000 14.03
ATOM	2060	CB	TRP	297 7.908		2159	102 137 320
ANISOU	2060	CB	TRP	297 1130	3.847	37.928	1.000 13.68
ATOM	2061	ĊĠ	TRP	297 8.646	1692	2376	-19 -169 1 5 1
ANISOU	2061	CG	TRP	297 1143	3.455	39.166	1.000 13.28
ATOM	2062	CD1	ממת		1646	2255	91 -96 2 2
ANISOU	2062	CD1	ממיז	297 8.932	2.179	39.622	1.000 15.58
ATOM	2063	CDJ	UDD TVE	297 1615	1689	2618	275 -544 - 77
ANISOU	2063	CD2	TKP	297 9.144	4.353	40.189	1.000 14.69
ATOM	2064	ND2	TRP	297 1327	1693	2562	<b>-1</b> 17 <b>-2</b> 19 5
ANISOU	2004	NEI	TRP	297 9.583	2.265	40.840	1.000 15.34
ATOM	2004	MET	TRP	297 1378	1853	2598	70 -494 7 5
ANTCOU	2065	CE2	TRP	297 9.724	3.597		1.000 16.13
ANISOU ATOM	2005	CE2	TRP	297 1241	2009	2880	182 -676 - 196
	2066	CE3	TRP	297 9.094	5.756	40.284	1.000 22.13
ANISOU	2066	CE3	TRP	297 3040	1658	3712	-665 -1408 129
ATOM	2067	CZ2	TRP	297 10.318	4.180		1.000 18.45
ANISOU	2067	CZ2	TRP	297 2204	2387	2418	
MOTA	2068	CZ3	TRP	297 9.670	6.353	11 300	44 -326 -331 1.000 21.55
ANISOU	2068	CZ3	TRP	297 2916	2104	3167	1.000 21.55
ATOM	2069	CH2	TRP	297 10.258	5.546		-55 -752 - 458
ANISOU	2069	CH2	TRP	297. 3298	2356	3205	1.000 23.53
ATOM	2070	N	ILE	298 5.106		3285	-320 -1146 -344
ANISOU	2070	N	ILE	298 1324	4.167 1726	39.044	1.000 13.58
ATOM	2071	CA	ILE	298 4.299		2108	241 -167 1 2 7
ANISOU	2071	CA	ILE	298 1413	4.440	40.229	1.000 14.68
MOTA	2072	Ċ	ILE	298 2.841	2177	1986	-13 -161 - 208
ANISOU	2072	č	ILE	298 1455	4.054	40.121	1.000 12.02
ATOM	2073		ILE		1300	1813	56 -239 402
ANISOU	2073	Õ	ILE	298 2.182	3.782	41.147	
ATOM	2074		ILE	298 1732	1582	1881	-23 -4 1 9 3
ANISOU	2074	CB		298 4.428	5.914	40.673	1.000 19.45
	, _	CD	ILE	298 2261	2446	2683	-699 237 -835

				-01-	
ATOM	2075 CG1	ILE	298 5.907	6.245	41.001 1.000 27.83
	2075 CG1		298 2776	4275	3525 -1314 -956 - 1030
ATOM	2076 CG2		298 3.679	6.319	41.929 1.000 25.05
	2076 CG2		298 3770	3344	2405 -57 255 -983
ATOM	2077 CD1		298 6.368	5.628	42.306 1.000 43.32
	2077 CD1		298 4561	7224	4674 -652 -1890 -117
ATOM	2078 N	GLY	299 2.317	3.980	38.893 1.000 12.16
ANISOU		GLY	299 1432	1308	1879 78 -304 106
ATOM	2079 CA	GLY	299 0.918	3.741	38.670 1.000 12.98
	2079 CA	GLY	299 1276	1279	2379 106 -188 - 154
ATOM	2080 C	GLY	299 0.135	5.017	38.378 1.000 13.09
ANISOU		GLY	299 1421	1403	2151 113 -231 1 1 8
ATOM	2081 0	GLY	299 0.738	6.025	38.017 1.000 14.00
ANISOU		GLY	299 1713	1353	2252 122 289 - 1 3
ANISOU	2082 N	GLY	300 -1.183	4.917	38.447 1.000 13.08
ANISOU		GLY	300 1325	1545	2099 146 -267 ~ 145
ATOM	2082 N 2083 CA	GLY	300 -2.075	5.966	37.992 1.000 13.45
ANISOU	2083 CA	GLY	300 -2.073	1521	2143 116 -415 -143
ATOM	2084 C	GLY	300 -2.519	6.972	39.042 1.000 12.94
ANISOU		GLY	300 1098	1365	2456 -52 -407 - 192
MOTA	2085 0	GLY	300 -3.262		38.672 1.000 13.39
ANISOU		GLY	300 1321	1342	2423 -19 -217 - 4 5
ANISOU	2085 N	ASN	301 -1.973	6.845	40.254 1.000 13.35
ANISOU		ASN	301 1494	1429	2151 -225 -232 -104
ANISOU	2080 N 2087 CA	ASN	301 -2.162	7.842	41.313 1.000 13.83
	2087 CA	ASN	301 1590	1435	2230 -194 -38 - 61
MOTA	2088 C	ASN	301 -0.837	8.254	41.885 1.000 12.46
ANISOU		ASN	301 -0.657	1268	1791 -35 -142 - 20
ATOM	2089 0	ASN	301 -0.007	7.405	42.169 1.000 13.89
	2089 0	ASN	301 1831	1355	2093 73 -144 - 13
ANISOU	2000 CB	ASN	301 -3.075	7.238	42.360 1.000 16.01
ANISOU	2090 CB	ASN	301 1632	1909	
ANISOU	2091 CG	ASN	301 -3.942	8.199	43.106 1.000 18.23
	2091 CG	ASN	301 1986	2508	2435 190 152 - 90
ATOM	2092 OD1		301 -4.973		42.614 1.000 17.44
	2092 OD1		301 1606	1626	3394 -21 144 -190
ATOM	2093 ND2		301 -3.518	8.454	44.338 1.000 33.30
	2093 ND2		301 2804	6923	2928 1012 -230 -1523
ATOM	2094 N	TYR	302 -0.595	9.564	42.073 1.000 12.96
	2094 N	TYR	302 1662	1278	1985 -69 -21 -135
ATOM	2095 CA	TYR	302 0.674	9.948	42.702 1.000 13.48
ANISOU		TYR	302 1673	1259	2192 -130 -132 3 4
ATOM	2096 C	TYR	302 0.768	9.269	44.078 1.000 12.63
	2096 C	TYR	302 1413	1293	2092 53 44 1 9
ATOM	2097 0	TYR	302 -0.218	9.151	44.806 1.000 14.15
ANISOU		TYR	302 1332	1737	2305 -65 48 - 27
ATOM	2098 CB	TYR	302 0.764	11.472	42.916 1.000 13.30
	2098 CB	TYR	302 1635	1192	2226 -81 33 4 1
ATOM	2099 CG	TYR	302 1.159	12.143	41.619 1.000 12.02
	2099 CG	TYR	302 1586	1103	1880 -59 -25 -271
ATOM	2100 CD		302 2.501	12.233	41.275 1.000 13.11
	2100 CD		302 1633	1284	2066 -80 11 -18
ATOM	2101 CD		302 0.235	12.709	40.739 1.000 12.52
	2101 CD		302 1576	1132	2049 -44 13 -127
ATOM	2102 CE		302 2.933	12.822	40.119 1.000 12.29
	2102 CE		302 1581	1043	2045 -185 -84 - 77
ATOM	2103 CE		302 0.637	13.273	39.535 1.000 14.12
	2103 CE		302 1462	1443	2458 -241 15 3 2 5
ATOM	2104 CZ		302 1.983	13.347	39.241 1.000 12.69
	7 2104 CZ		302 1483	1224	2113 -287 -91 1 0
ATOM	2105 OH		302 2.376	13.866	
			-		

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ANISO	U 210	5 OH	TYR	30	2 1505	1469	2124	
ATOM	210	бΝ	VAL		3 1.956	8.855	2124	-93 33 1 4 6
ANISO			VAL	3 0	3 1406	1637	44.450	0 1.000 1392
ATOM	210	7 CA	VAL		3 2.355	8.336	2246	153 88 9 9
ANISO	U 210	7 CA	VAL	3.0	3 1838		45.746	6 1.000 14.51
ATOM	210	8 C	VAL	30	3 3.498	1320	2355	-137 -391 - 74
ANISO	U 210	8 C	VAL	30	3 1404	9.244	46.239	9 1.000 15.23
ATOM	210	9 0	VAL	30.	3 4.471	1507	2876	-102 -105 -340
ANISO	U 210	9 0	VAL	30.	3 1859	9.386	45.512	2 1.000 18.70
ATOM		O CB	VAL	30.	3 2.856	1861	3386	-239 326 -504
ANISO	J 211	O CB	VAL	303	3 2140	6.880	45.632	2 1.000 16.75
ATOM	211	l CG	l VAL		3.279	1319	2905	16 - 759 - 123
ANISO	J 211	L CG	VAL	302	3.279	6.401	47.017	1.000 19.53
ATOM	2112	2 CG	VAL	302	3 1.723	1951	3284	232 -1054 148
ANISOU	J 2112	2 CG2	VAT.	302	2476	5.956	45.125	1.000 17.82
MOTA	211:	3 N	ASN	303	3.349	1442	2852	-213 -558 - 406
ANISOU	J 211	3 N	ASN	304	1409	9.900	47.378	1.000 14.07
ATOM		CA	ASN	304	4.317	1369	2566	-39 -407 - 86
ANISOU	7 2114	CA	ASN	304	1474	10.928	47.772	1.000 14.31
ATOM	2115		ASN		5.450	1387	2578	-102 -424 - 55
ANISOU	J 2115	Ċ	ASN	304	1360	10.397	48.637	1.000 13.75
ATOM	2116	0	ASN	304	6.539	1487	2378	34 - 274 - 87
ANISOU	2116	0	ASN	304	1314	10.962	48.584	1.000 14.60
ATOM	2117		ASN	304	3.589	1795	2438	-34 -55 -32n
ANISOU	2117	CB	ASN	304	3.589 1710	12.035	48.551	1.000 14.26
ATOM	2118	CG	ASN	304	2.535	1214	2494	6 -303 176
ANISOU	2118	CG	ASN	304	1551	12.661	47.642	1.000 14.81
ATOM	2119	ומס	ASN	304	2.866	1627	2449	23 -114 402
ANISOU	2119	001	ASM	304	1896	13.255	46.622	1.000 16.52
$\mathtt{ATOM}$	2120	ND2	ASM	304	1.290	1746	2636	80 19 5 8 9
ANISOU	2120	ND2	ASN	304	1560	12.595	48.102	1.000 18.43
ATOM	2121	"N	ILE		5.175	2980	2463	127 -10 199
ANISOU	2121	N	ILE	305	1546	9.413	49.463	1.000 16.36
ATOM	2122	CA	ILE	305	6.173	1553	3117	-78 -503 2 6 6
ANISOU	2122	CA	ILE	305	1670	8.890	50.407	1.000 14.85
ATOM	2123	C	ILE	305	6.183	1537	2436	165 -277 - 40
ANISOU	2123	Č	ILE	305	1527	7.372	50.352	
ATOM	2124	Õ	ILE	305	5.231	1555	2914	95 -438 - 51
ANISOU	2124	Ō	ILE	305	1463	6.736	49.886	1.000 17.54
ATOM	2125	CB	ILE	305	5.949	1789	3412	-131 -404 5
ANISOU	2125	CB	ILE	305	2167	9.430	51.818	1.000 17.80
$\mathtt{MOTA}$	2126	CG1	TLF	305	4.578	1962	2634	-23 265 -209
ANISOU	2126	CG1	ILE		1716	9.091 2948	52.416	1.000 18.93
ATOM	2127	CG2	TLE	305	6.171	10.944	2526	1 -218 -163
ANISOU	2127	CG2	ILE	305	2685		51.823	1.000 19.17
ATOM	2128	CD1	ILE	305	4.415	1863	2737	70 -534 -405
ANISOU	2128	CD1	ILE	305	2521	9.459 2902	53.863	1.000 21.28
ATOM	2129	N	ARG	306	7.246	6.806	2662	19 452 - 71
ANISOU	2129	N	ARG	306	1738		50.908	1.000 14.59
ATOM	2130	CA	ARG		7.424	1641	2165	52 -356 271
ANISOU	2130	CA	ARG	306	1509	5.360 1663	50.828	1.000 15.25
ATOM	2131	С	ARG	306	8.234		2622	139 -302 7 7
NOSINA	2131	С	ARG	306	1588	4.903	52.024	1.000 15.02
ATOM	2132	0	ARG	306	9.141	1464	2656	133 -332 - 21
ANISOU	2132	Ō	ARG	306	1682	5.614	52.433	1.000 16.63
ATOM	2133	CB	ARG	306	8.135	2101	2536	-219 -294 -168
ANISOU	2133		ARG	306	1820	4.943	49.532	1.000 16.31
ATOM	2134	CG	ARG	306	8.226	1681	2697	-100 -270 -150
ANISOU	2134		ARG		2476	3.414	49.377	1.000 18.43
ATOM	2135	CD	ARG	306	8.401	1700	2828	40 -194 -156
ANISOU	2135		ARG	306	2087	3.068	47.900	1.000 18.26
	200			200	200/	1971	2880	-120 -145 - 330

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ATOM	2136	NE	ARG	306	7.136	3.228	47.188	1.000	20.53
ANISOU	2136	ΝE	ARG		2442	2013			-16 <del>6</del> 3 - 234
ATOM	2137		ARG		6.980	3.178	45.873	1.000	20.27
ANISOU	2137	CZ	ARG	306	2330	2057	3316	373	-522 2 0
ATOM	2138			306	8.086	3.000	45.107		
ANISOU					2136	2580			-589 - 723
ATOM	2139				5.759	3.250	45.341		
ANISOU					2107	1838			-285 8 4
ATOM	2140		ARG		7.898	3.775	52.612		
ANISOU			ARG		2716	1872			-607 3 2 7
ATOM	2141		ARG		8.576	3.212	53.768		
ANISOU			ARG		3321	2201			-845 1 3 9
ATOM	2142		ARG		9.536	2.138	53.277		
ANISOU	2142		ARG		3417	2170			-1046 3 9
ATOM	2143	-	ARG		9.385	1.601	52.187		
ANISOU			ARG		2574	2355			-728 1 1 2
ATOM	2144		ARG		7.557	2.522	54.694		
ANISOU			ARG		4545	3184		-13	-247 7 0 5
ATOM	2145		ARG		6.839	3.488	55.629		
ANISOU			ARG		6310	6374		215	1655 - 970
ATOM	2146		ARG	307	7.054	3.085	57.085		
ANISOU			ARG		11107	10355			2792 - 1145
ATOM	2147		ARG		5.989	2.203	57.531		
ANISOU			ARG		11821	12833			1969 - 5
ATOM	2148		ARG		5.987	1.285	58.479		
ANISOU			ARG		7704	14382			1249 1051
ATOM	2149				7.063	1.038	59.214		
ANISOU					6613	17949	5955		2179 1 0 5
ATOM	2150				4.872	0.597	58.707		
ANISOU				307		15919	2983	-6954	
ATOM	2151		THR		10.551	1.861	54.113		
ANISOU			THR		4234	2212	3285	536	-1421 -232
ATOM	2152		THR		11.308	0.640	53.822		
ANISOU			THR		3468	1939	5998	225	-1629 - 194
MOTA	2153		THR		10.468	-0.611	54.030		
ANISOU			THR		2915	2190	4552	453	-626 -321
ATOM	2154		THR		9.523	-0.768	54.787	1.000	
ANISOU			THR		4042	3482	3912	614	-217 -125
ATOM	2155		THR		12.581	0.531	54.688		
ANISOU			THR		2701	3586	3626	242	-361 -456
ATOM			THR		12.140	0.751	56.028		32.90
ANISOU			THR		4146	4188	4167	504	745 - 495
ATOM			THR		13.577	1.594			31.43
ANISOU					3193	4702	4047	-577	-132 -538
ATOM	2158		SER		10.850	-1.591			24.73
ANISOU			SER		2934	2092	4370	94 -5	74 - 391
ATOM	2159		SER		10.199	-2.897	53.230	1.000	25.19
ANISOU			SER		3793	2464	3316	-485	451 - 230
ATOM	2160		SER		10.466	-3.691			24.06
ANISOU			SER		2360	2888	3893	302	107 3 5
ATOM	2161		SER		11.565	-3.621	55.084		34.54
ANISOU			SER		3626	2131	7366	-76	-1944 - 34
ATOM	2162		SER		10.639	-3.700	52.012		26.52
ANISOU			SER		3970	2159	3948	167	580 - 366
ANISOC	216		SER		9 10.217	-5.039	52.148		26.34
ANISOU			SER		3198	2207	4604	156	-844 - 260
ATOM	216		LYS		0 9.494	-4.458			24.99
ANISOU			LYS		0 3172	2459	3864	160	262 366
ATOM		5 CA			0 9.651	-5.339			28.38
ANISO					0 4191	3167	3427	764	278 281
ANISO	216		LYS		0 9.941	-6.768			0 26.07
A TOM	210			71	· / . /	5.750			

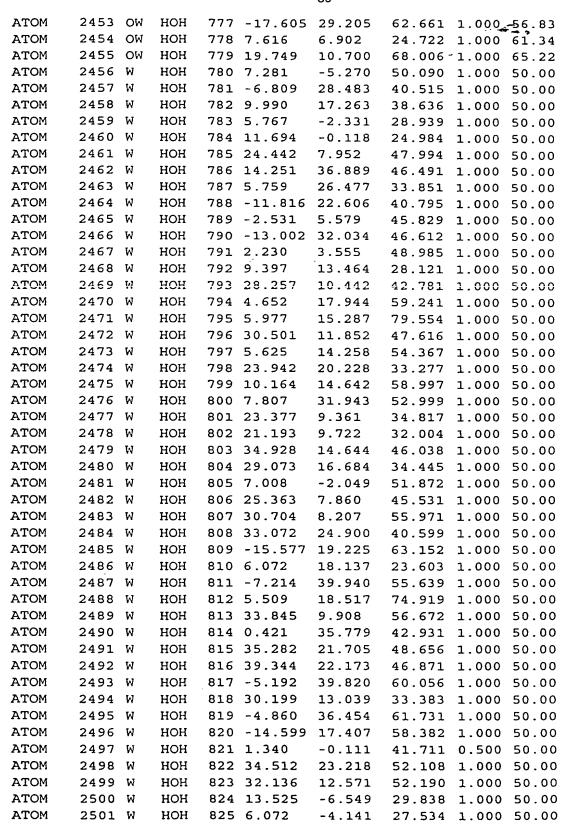
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ANISO			LYS		0 33	71	2687	3846	168	200 5 5 5
ATOM	216	7 0	LYS		0 10	.150	-7.684	56.51		-290 5 7 7 0·3 <del>-</del> 34 8
ANISOU ATOM			LYS		0 52	67	3056	4400	-66	-450 1073
ANISOU		8 CB 8 CB			0 8.2	299	-5.367		-00 } 1~0∩0	37.77
ATOM		9 CG	-	31	0 573	3 6	4695	3921	299	1818 1 8
ANISOU	7 2 1 6	9 CG	_	31	0 8.0	014	-4.214	57.806		0 40.55
ATOM	217	O CD	LYS LYS	31	639	95	4716	4295	1525	1524 1 0 1
ANISOU	7 217	0 CD	LYS	3 L	0 6.7	798	-4.587	58.649	1.000	) 44.24
ATOM	217	1 CE	LYS	31	909	71	4224	3495	1053	2816 5 9 4
ANISOU	217	1 CE	LYS	31	0 6.7 0 928	/ 22	-6.109		1.000	59.12
ATOM	217	2 NZ	LYS	31	6.0	) O O	4577	8606	766	-82 2478
ANISOU	217	2 NZ	LYS	310	488	100	-6.563 5742			55.80
ATOM	217	3 N	ALA		9.8		-7.030	10577	287	-947 4796
ANISOU			ALA	31	219	0	2402			1 2 2 . 4 5
ATOM	217	4 CA	ALA		10.		-8.369	3939	10 52	269
ANISOU	217	4 CA	ALA	311	377	1	2594	53.972	1.000	31.89
ATOM	2179	5 C	ALA		11.		-8.459	53.833	434	-516 - 421
ANISOU		5 ·C	ALA	311	390	7	2328	2616	1393	23.30
ATOM	2176	CB	ALA	311	9.6	19	-8.665		1 000	-593 1 1 2 27.94
ANISOU ATOM	2176	CB	ALA	311	240	7	2878	5329	-355	27.94 542 -672
ATOM	2177	OW	нон	501	-6.	477	10.237		1 000	542 - 672 15.66
ATOM	2178 2179	WO S	нон	502	-9.	349	16.189	51.010	1.000	19.26
ATOM	2180		НОН	503	-1.	489	3.653	34.560	1.000	15.78
ATOM	2181		нон нон	504	-10	.499	18.731	50.182	1.000	16.19
ATOM	2182		НОН	505	-8.	612	16.958	47.640	1.000	17.30
ATOM	2183		НОН	500	2.0	.255	20.839	42.881	1.000	19.05
ATOM	2184	OW	нон	507	-0.	96 204	1.076	32.810	1.000	29.32
ATOM	2185		нон	500	-8.	284 505	4.743	41.885	1.000	13.93
ATOM	2186	OW	нон	510	3.1	525 65	18.553	42.416	1.000	21.33
ATOM	2187	WO	нон	511	-6.	282	2.604 19.386	43.488	1.000	
ATOM	2188		нон	512	-6.8	826	24.638	52.341	1.000	18.98
ATOM	2189	OW	HOH	513	10.5	510	-4.344	46.833	1.000	21.77
ATOM	2190	OW	нон	514	-0.8	306	16.964	46.092	1.000	25.88
ATOM	2191	OW	нон	515	-1.2	269	18.855	40.372 42.411		
ATOM	2192		нон	516	14.2	277	-5.146	40.175	1 000	15.76
ATOM ATOM	2193	OW	нон	517	-0.1	123	21.538	40.640	1 000	17 22
ATOM	2194	OW	нон	518	13.1	L31	-0.967	51.791	1 000	11.22
ATOM	2195 2196	OW	нон	519	11.0	009	2.875	45.599	1.000	20 20
ATOM	2197		НОН	520	5.78	39	13.543	45.996	1.000	17 36
	2198	OW	нон нон		2.16		19.767	55.925	1.000	20.41
	2199	OW เพ	НОН	522	8.48	37	15.960	34.949	1.000	15.40
ATOM	2200	WO	нон	524	10.7	794	12.697	29.921	1.000	19.99
ATOM	2201	OW	нон	525	1.67	122	19.112	44.516	1.000	19.82
ATOM	2202	OW	нон	526	9.65	12	-2.081	35.124	1.000	16.29
ATOM	2203	OW	нон	527	28.7	7/10	15.283 31.187	32.342	1.000	20.37
ATOM	2204	OW	нон	528	15.3	26	11.252	52.019	1.000	18.53
ATOM	2205	OW	HOH	529	26.8	97	26.984	32.041	1.000	19.60
ATOM	2206	OW	HOH	530	13.5	28	11.592	52.035	1.000	19.86
ATOM	2207	OW	нон	531	25.6	31	32.409	50.915	T.000	16.17
ATOM	2208	OW	нон	532	18.2	87	6.835	52.682	1.000	19.20
ATOM	2209	OW	нон	533	12.6	35	29.035	52.185 39.395	1 000	18.49
ATOM	2210	OW	НОН	534	10.7	97	31.968	45.659	1 000	18.09
ATOM ATOM	2211	OW	нон	535	10.1	67	24.890	33.567	1 000	20.00 10 10
	2212	OM	нон	536	23.5	30	24.122	58.531	1 000	17.14 20 30
	2213 2214	OW	нон	537	23.3	58	12.639	35.292	1.000	20.33
	2214	OW.	HOH	538	25.8	79	28.699	50.264	1.000	19.44
ATOM	2215		HOH	539	11.6		16.559	30.502	1.000	18.57
	10	O W	НОН	540	18.5	15	27.775	40.042	1.000	22.23
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2 50 21	2217 00		5.1. 0.1 0.2.2	- 00 -	
ATOM	2217 OW	нон	541 21.233	20.367	33.996 1.000 21.45
ATOM	2218 OW	нон		32.643	53.094 1.000 19-38
ATOM	2219 OW	нон	543 19.670	22.387	35.310 1.000 20.05
ATOM	2220 OW	нон	544 -13.591		61.494 1.000 49.93
MOTA	2221 OW	нон	545 21.295	11.783	55.080 1.000 20.04
MOTA	2222 OW	нон	546 5.431	2.533	51.677 1.000 28.11
ATOM	2223 OW	нон		25.489	32.148 1.000 24.38
ATOM	2224 OW	нон	548 17.427	7.744	33.008 1.000 20.78
MOTA	2225 OW	нон	549 11.656	23.874	58.194 1.000 23.39
ATOM	2226 OW	нон	550 8.037	14.987	53.326 1.000 33.52
ATOM	2227 OW	нон	551 1.354	14.574	33.889 1.000 21.05
ATOM	2228 OW	нон		20.116	63.686 1.000 24.59
ATOM	2229 OW	нон	553 2.671	21.240	34.245 1.000 34.51
ATOM	2230 OW	нон	554 6.339	19.832	30.751 1.000 26.36
ATOM	2231 OW	нон	555 26.611	24.519	55.570 1.000 21.22
ATOM	2232 OW	нон	556 27.669	17.156	53.039 1.000 25.86
ATOM	2233 OW	нон	557 -14.392		44.154 1.000 25.03
ATOM	2234 OW	нон		32.652	51.443 1.000 25.23
MOTA	2235 OW	нон		7.207	54.915 1.000 20.59
ATOM	2236 OW	НОН	560 10.729	-8.875	31.499 1.000 24.65
MOTA	2237 OW	нон	561 6.455	2.298	42.613 1.000 22.74
ATOM	2238 OW	нон	562 13.784	31.245	44.166 1.000 27.75
MOTA	2239 OW	нон	563 17.292	33.470	53.556 1.000 25.28
ATOM	2240 OW	нон	564 11.210	1.109	49.697 1.000 23.33
MOTA	2241 OW	НОН	565 -11.339		41.370 1.000 26.08
MOTA	2242 OW	нон	566 20.363	-8.375	38.242 1.000 30.07
MOTA	2243 OW	нон	567 3.890	24.604	35.837 1.000 25.86
MOTA	2244 OW 2245 OW	НОН	568 5.334	11.875	43.937 1.000 25.45
MOTA MOTA	2245 OW 2246 OW	НОН	569 7.861	22.385	64.046 1.000 28.98
ATOM	2240 OW 2247 OW	HOH	570 7.754	-1.508	30.848 1.000 24.72
ATOM	2247 OW 2248 OW	НОН	571 6.297	3.583	28.471 1.000 33.06
ATOM	2248 OW 2249 OW	нон нон	572 -15.790 573 -5.388		51.855 1.000 30.09
ATOM	2249 OW 2250 OW	нон		20.310	38.883 1.000 23.64
ATOM	2250 OW 2251 OW	нон		21.059	29.053 1.000 24.31
ATOM	2251 OW 2252 OW	НОН	575 8.763 576 10.135	20.920	66.102 1.000 24.81
ATOM	2252 OW 2253 OW	нон	576 10.135	27.617	58.357 1.000 25.12
ATOM	2254 OW	нон	578 22.601	1.060	29.730 1.000 29.00
MOTA	2255 OW	нон	579 8.859	4.744	61.946 1.000 28.66 27.898 1.000 26.12
ATOM	2256 OW	нон	580 4.937	3.932	48.882 1.000 26.29
ATOM	2257 OW	нон	581 17.096	5.891	35.057 1.000 23.31
ATOM	2258 OW	нон	582 -16.337		
ATOM	2259 OW	нон	583 7.652	24.826	52.106 1.000 27.23
ATOM	2260 OW	нон	584 7.174	24.915	29.292 1.000 26.60
ATOM	2261 OW	нон	585 23.452	10.614	55.439 1.000 26.42
ATOM	2262 OW	нон	586 12.640	26.413	58.676 1.000 27.15
ATOM	2263 OW	нон	587 6.204	21.166	62.094 1.000 24.65
ATOM	2264 OW	нон	588 2.385	0.810	37.616 1.000 19.92
ATOM	2265 OW	нон	589 32.930	28.236	45.738 1.000 38.29
ATOM	2266 OW	нон	590 -12.045		45.065 1.000 30.46
ATOM	2267 OW	нон	591 0.219	13.612	36.120 1.000 27.12
ATOM	2268 OW	нон	592 -2.525	3.881	43.344 1.000 26.67
MOTA	2269 OW	нон	593 7.533	13.297	48.055 1.000 19.59
ATOM	2270 OW	нон	594 -1.575	28.355	42.057 1.000 25.53
ATOM	2271 OW	нон	595 11.209	-1.188	46.425 1.000 22.12
ATOM	2272 OW	нон	596 5.684	-7.000	28.451 1.000 27.97
MOTA	2273 OW	нон	597 28.868	19.406	51.825 1.000 27.72
ATOM	2274 OW	нон	598 13.432	2.493	57.904 1.000 31.12
ATOM	2275 OW	нон	599 8.196	7.483	27.148 1.000 29.99
ATOM	2276 OW	нон	600 20.809	19.088	63.369 1.000 36.86
ATOM	2277 OW	нон	601 21.352	10.656	34.614 1.000 30.60

- 87 -MOTA 2339 OW HOH 663 19.354 0.465 27.273 1.000 44.56 ATOM 2340 OW нон 664 24.969 27.026 38.838 1.000 35 ±1 ATOM 2341 OW нон 665 24.294 7.488 55.914 1.000 32.97 2342 OW ATOM HOH 666 19.540 7.882 31.178 1.000 30.04 **ATOM** 2343 OW нон 667 -9.236 32.988 57.241 1.000 39.20 MOTA 2344 OW нон 668 2.098 18.351 67.496 1.000 38.83 ATOM 2345 OW HOH 669 11.390 3.245 56.270 1.000 37.56 ATOM 2346 OW нон 670 -21.413 24.449 52.026 1.000 44.66 ATOM 2347 OW 671 -14.575 19.220 55.240 1.000 30.91 HOH MOTA 2348 OW нон 672 32.112 25.958 43.051 1.000 33.34 MOTA 2349 OW нон 673 -15.050 31.151 53.232 1.000 34.71 2350 OW MOTA 674 2.941 HOH -1.607 30.245 1.000 34.63 2351 OW ATOM 14.544 34.757 1.000 49.17 30.669 39.386 1.000 30.55 18.009 68.080 1.000 43.41 675 26.951 HOH ATOM 2352 OW 676 14.707 нон 30.669 677 5.203 ATOM 2353 OW НОН 2354 OW 678 14.151 ATOM HOH 7.965 26.591 1.000 38.80 24.261 41.443 1.000 31.28 2.410 28.478 1.000 34.31 20.593 34.326 1.000 39.66 35.357 44.421 1.000 34.06 2.355 45.456 1.000 35.39 34.538 42.053 1.000 33.55 2355 OW MOTA 679 24.470 нон MOTA 2356 OW нон 680 17.540 ATOM 2357 OW HOH 681 25.992 MOTA 2358 OW HOH 682 13.802 2359 OW 683 1.087 MOTA HOH 2360 OW MOTA нон 684 22.443 27.356 1.000 48.02 51.877 1.000 50.63 MOTA 2361 OW HOH 685 4.419 4.720 2362 OW ATOM нон 686 -15.830 34.507 2363 OW MOTA 687 -15.217 29.490 HOH 48.887 1.000 33.54 MOTA 2364 OW HOH 688 36.808 21.183 46.206 1.000 44.97 MOTA 2365 OW нон 689 3.756 1.312 29.272 1.000 35.16 MOTA 2366 OW нон 690 18.802 13.646 27.901 1.000 30.08 2367 OW MOTA HOH 691 6.997 17.521 29.313 1.000 47.70 2368 OW ATOM 692 13.725 нон 16.327 69.105 1.000 36.97 ATOM 2369 OW нон 693 22.369 22.161 60.503 1.000 44.09 MOTA 2370 OW нон 694 -5.429 31.620 42.219 1.000 33.40 MOTA 2371 OW 695 19.351 HOH 23.082 30.744 1.000 34.21 2372 OW ATOM нон 696 6.897 22.414 29.376 1.000 36.59 MOTA 2373 OW нон 697 28.700 7.809 57.304 1.000 38.35 MOTA 2374 OW HOH 698 3.224 0.679 39.819 1.000 24.13 2375 OW MOTA HOH 699 -4.634 33.717 62.593 1.000 32.26 2376 OW MOTA 703 -11.313 34.067 46.117 1.000 49.40 704 7.774 31.390 65.371 1.000 39.75 705 24.764 7.530 36.000 31.75 700 32.423 HOH 17.018 43.200 1.000 43.20 2377 OW MOTA HOH MOTA 2378 OW HOH ATOM 2379 OW HOH ATOM 2380 OW HOH 705 24.764 7.530 36.802 1.000 38.55 706 -22.095 25.669 59.047 1.000 36.71 MOTA 2381 OW нон MOTA 2382 OW HOH MOTA 2383 OW 707 14.509 9.840 HOH 68.854 1.000 50.38 708 -10.129 28.722 42.036 1.000 38.92 ATOM 2384 OW HOH MOTA 2385 OW 709 29.011 HOH 34.910 48.390 1.000 35.29 ATOM 2386 OW 710 15.822 HOH 31.612 42.021 1.000 33.61 33.645 1.000 49.57 26.015 1.000 41.04 37.371 1.000 43.47 35.599 1.000 45.99 ATOM 2387 OW 711 -1.996 17.676 НОН MOTA 2388 OW нон 712 10.216 17.748 MOTA 2389 OW нон 713 23.535 29.642 MOTA 2390 OW 714 20.488 нон -7.214 ATOM 2391 OW 715 11.411 нон 10.149 25.081 1.000 41.63 ATOM 2392 OW нон 716 19.329 -4.258 34.139 1.000 42.50 ATOM 66.321 1.000 43.74 54.747 1.000 40.47 2393 OW нон 717 13.688 26.799 ATOM 2394 OW 718 -10.751 33.064 HOH ATOM 2395 OW 719 13.800 18.258 нон 70.756 1.000 34.54 ATOM 2396 OW 720 17.151 HOH 5.815 28.003 1.000 40.80 ATOM 2397 OW нон 721 0.000 0.000 36.691 0.330 27.42 MOTA 2398 OW HOH 722 0.000 0.000 41.559 0.330 37.77 MOTA 2399 OW нон 723 15.314 7.549 28.791 1.000 36.24

					00 -			
ATOM	2400 (	нон ис	724	-1.663	19.944	39.196	1.000	33.87
ATOM	2401 (	HOH WC	725	19.289	24.195	33.321		32.28
ATOM	2402 (	HOH WC	726	0.000	0.000	31.798		
ATOM	2403 (	HOH WC	727	-1.223	38.165	59.229		31.24
ATOM		HOH WC	728	22.035	38.254	45.742		48.21
MOTA	2405 (	HOH WC	729	28.388	16.248	63.044		
MOTA	2406 C	HOH WC	730	0.000	0.000	45.995		
ATOM	2407 C	HOH WC	731	2.984	29.007	40.091		36.08
MOTA	2408 C	HOH WC	732	5.297		27.318		41.53
MOTA	2409 C	HOH WC	733	17.347	10.778	27.373		35.27
MOTA	2410 C	HOH W	734	29.417	14.607	53.127		40.12
MOTA		HOH W	735	4.222	-8.636	27.012		35.22
ATOM	2412 C	HOH W	736	-9.949	17.712	62.813		34.43
ATOM		HOH W	737	13.960	-10.203	55.259	1.000	31.79
ATOM		HOH W	738	11.831	-1.522	49.308		
ATOM	2415 C	HOH W	739	2.896	4.247	29.596		38.64
MOTA	2416 C	HOH W	740	10.959	13.759	25.528		
ATOM	2417 O	HOH W	741	0.864	17.227	30.557		
ATOM	2418 C	HOH W	742	31.755	18.949		1.000	
MOTA	2419 O	HOH W	743	21.678	-0.485	28.218		43.23
ATOM	2420 O	HOH W	744	10.583	16.397	75.211	1.000	
MOTA	2421 0	HOH W	745	7.480	7.996	78.287	1.000	
MOTA	2422 0	HOH W	746	24.067		40.297	1.000	
MOTA	2423 O	HOH W	747	7.804	10.269	78.332	1.000	
MOTA	2424 O	HOH W	748	22.131		45.806	1.000	
MOTA	2425 <sub>.</sub> 0		749	14.850	-4.647	33.872		42.88
MOTA	2426 O	HOH W	750	-12.930	32.504	55.211		37.15
ATOM	2427 O	W HOH	751	-4.832	35.986	43.333	1.000	
MOTA	2428 O	W HOH	752	19.834	33.566	56.449	1.000	31.56
ATOM	2429 O	M HOH	753	3.363	22.310	29.844	1.000	42.02
ATOM	2430 O	W HOH	754	25.594	4.030	34.174	1.000	51.90
ATOM	2431 O	HOH W	755	28.036	35.859	46.448	1.000	
ATOM	2432 0	W HOH	756	-12.951	16.294	61.787	1.000	
ATOM	2433 O	W HOH	757	-10.870	26.452	38.737	1.000	
MOTA	2434 0	HOH W	758	13.216	12.896	70.729	1.000	
MOTA	2435 O	W HOH	759	-0.403	21.161	74.990		
ATOM	2436., O	W HOH	760	-7.025	32.526	64.316		
MOTA	2437 O	HOH W	761	-15.459	19.739		1.000	
MOTA	2438 O	HOH W	762	-4.964	36.577		1.000	
MOTA	2439 O	HOH W	763	26.807	35.717		1.000	
MOTA	2440 O	HOH W	764	19.542	7.083	65.538		41.41
ATOM	2441 0	HOH W	765	3.709	35.837	42.709		33.78
MOTA	2442 0	W HOH	766	0.431	33.688	40.172	1.000	
MOTA	2443 O	HOH W	767	18.620	5.064	64.617	1.000	
MOTA	2444 0	HOH W	768	35.526	19.792	41.322	1.000	
ATOM	2445 O	W HOH	769	19.671	7.789	67.717	1.000	
MOTA	2446 O	и нон	770	3.562	12.048	26.149	1.000	
ATOM	2447 0	и нон	771	20.245	35.637		1.000	
MOTA	2448 O	и нон	772	-20.588	25.640	61.573	1.000	
ATOM	2449 O	HOH W	773	1.556	37.342	52.171		36.23
MOTA	2450 O	и нон	774	8.340	0.668	49.382	1.0001	
ATOM	2451 O	и пон	775	27.160	2.372	34.466	1.000	
MOTA	2452 O	м нон	776	6.575	19.271	25.545	1.000	



## STRUCTURE B

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ATOM	1	CB	MET	1	31.030	11.882	57.066	1.000 50.96
ANISOU	Jl	CВ	MET	1	5663	3892	9809	1113 -2217 -554
ATOM	2	CG	MET	1	30.206	12.690	56.086	1.000 51.63
ANISOU	J 2	CG	MET	1	6595	3775	9246	
ATOM	3	SD	MET	ī				691 -1891 169
ANISOU		SD			28.694	11.848	55.559	1.000 40.50
			MET	1	7003	3962	4424	833 -1535 -460
ATOM	4	CE	MET	1	27.852	11.584	57.120	1.000 45.32
ANISOU		CE	MET	1	8632	3912	4677	-239 -653 -1702
ATOM	5	С	MET	1	31.587	13.367	58.999	1.000 52.14
ANISOU	15	С	MET	1	6204	4752	8854	
ATOM	6	0	MET	1	31.239	12.847	60.058	
ANISOU	1 6	Ö	MET	ī	7381			1.000 52.92
ATOM	7	N	MET	i		5242	7483	1417 -4224 519
ANISOU					33.170	11.646	58.275	1.000 57.78
		N	MET	1	4533	6034	11388	34 -1912 - 811
ATOM	•	CA	MET	1	32.156	12.587	57.819	1.000 54.62
ANISOU		CA	$\mathtt{MET}$	1	6441	4752	9560	137 -2012 -617
$\mathtt{ATOM}$	9	N	ASP	2	31.485	14.679	58.792	1.000 43.52
ANISOU	9	N	ASP	2	3460	4866	8210	
ATOM	10	CA	ASP	2	30.759			474 -2350 4 7
ANISOU		CA	ASP	2		15.471	59.796	1.000 41.69
ATOM	11				4439	4678	6722	-309 -2603 - 31
		CB	ASP	2	31.206	16.912	59.644	1.000 37.89
ANISOU		СВ	ASP	2	3805	4768	5822	-304 -3473 266
MOTA	12	CG	ASP	2	30.219	17.958	60.121	1.000 39.59
ANISOU	12	CG	ASP	2	4511	4616	5916	15 -3218 5 8 9
ATOM	13	OD1	ASP	2	29.325		60.933	1 000 45 70
ANISOU	13		ASP	2	5866	4689		1.000 45.10
ATOM	14		ASP	2			6581	-553 -1950 -625
ANISOU			ASP		30.363	19.121	59.663	1.000 42.05
				2	5994	4341	5643	-465 -3788 145
ATOM	15	Ç	ASP	2	29.275	15.213	59.556	1.000 33.84
ANISOU		C	ASP	2	4131	3634	5094	-59 -1682 -122
MOTA	16	0	ASP	2	28.901	15.176	58.379	1.000 29.25
ANISOU	16	0	ASP	2	2232	4393	4489	658 -390 - 615
ATOM	17	N	THR	3	28.467	15.029		
ANISOU		N	THR	3	4731		60.597	1.000 29.41
ATOM	18	CA	THR	3		2636	3807	907 -2076 -284
ANISOU					27.046	14.764	60.421	1.000 28.55
		CA	THR	3	4602	2494	3753	597 -1006 - 390
ATOM	19	CB	THR	3	26.447	13.762	61.414	1.000 36.51
ANISOU		CB	THR	3	7170	2209	4495	-791 -1996 5 2
ATOM	20		THR	3	26.629	14.220	62.758	1.000 42.45
ANISOU	20	OG1	THR	3	9519	2620	3989	-920 -1251 3 8 3
MOTA	21	CG2	THR	3	27.153	12.412	61.315	
ANISOU	21		THR	3	9604	1863		1.000 50.26
ATOM	22	Ċ	THR	3		1003	7630	-602 -733 - 333
ANISOU		-			26.240		60.553	1.000 29.01
ATOM		C	THR	3	4535	2548	3939	738 -1079 9 9
	23	0	THR	3	25.041	16.044	60.827	1.000 35.82
ANISOU		0	THR	3	5149	2485	5976	390 524 -1246
ATOM	24	N	THR	4	26.928	17.181	60.332	1.000 24.98
ANISOU	24	N	THR	4	3874	2456	3162	
ATOM	25	CA	THR	4	26.214			
ANISOU		CA	THR	4		18.465	60.327	1.000 23.97
ATOM					3437	2426	3244	344 -1563 - 375
	26	CB	THR	4	27.183	19.650	60.408	1.000 26.77
ANISOU		CB	THR	4	2636	2429	5105	651 -988 - 923
MOTA	27	OG1		4	28.050	19.484	61.551	1.000 32.62
ANISOU	27	OG1	THR	4	3398	2812	6184	
ATOM	28	CG2		4	26.429	20.942		
ANISOU		CG2		4	2373		60.663	1.000 26.40
ATOM	29	C				2692	4967	533 -573 -1570
ANISOU			THR	4	25.325	18.577	59.097	1.000 21.64
		C	THR	4	3090	2760	2374	368 -750 - 20
ATOM	30	0	THR	4	25.⁄ <b>7</b> 38	18.264		1.000 21.58
ANISOU		0	THR	4	2668	2629	2902	246 -560 - 659
MOTA	31	N	VAL	5	24.104	19.049	59.340	1.000 15.88
					- <del>-</del>			2.000 13.00

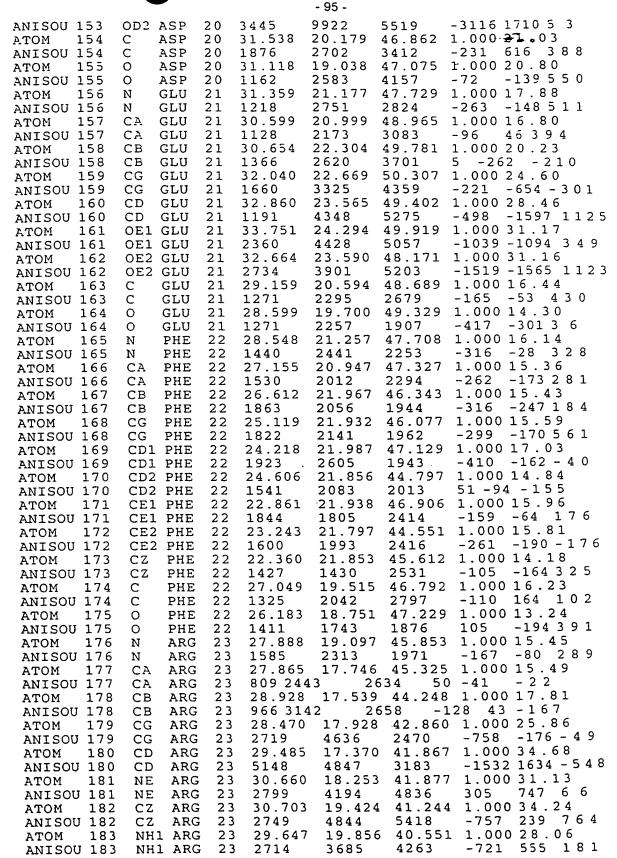
				- 31 -		
ANISOU 31	N VAL	5	2505	2021	1508	-613 -630 -162
ATOM 32	CA VAL	5	23.211	19.385	58.211	1.000 1-42.80
ANISOU 32	CA VAL	5	2463	1893	1266	-594 -473 - 87
ATOM 33	CB VAL	5	21.742	19.402	58.606	1.000 16.09
ANISOU 33	CB VAL	5	2476	1881	1757	-412 -406 5 0 2
ATOM 34	CG1 VAL	5	20.855	19.846	57.447	
ANISOU 34	CG1 VAL	5	2468			1.000 14.91
		5		1859	1337	9 -102 197
ATOM 35	CG2 VAL		21.310	17.994	59.074	1.000 21.15
ANISOU 35	CG2 VAL	5	3015	2345	2677	-700 -418 1198
ATOM 36	C VAL	5	23.639	20.762	57.694	1.000 17.70
ANISOU 36	C VAL	5	2893	2085	1749	-1137 -713 1 0 3
ATOM 37	O VAL	5	23.532	21.759	58.419	1.000 17.35
ANISOU 37	O VAL	5	2566	1978	2050	-698 -650 1 0 5
ATOM 38	N PRO	6	24.150	20.845	56.479	1.000 13.23
ANISOU 38	N PRO	6	1334	1597	2097	-162 -668 4 0 9
ATOM 39	CD PRO	6	24.302	19.770	55.484	1.000 15.56
ANISOU 39	CD PRO	6	1887	1850	2176	-309 -383 2 7 7
ATOM 40	CA PRO	6	24.667	22.137	56.005	1.000 14.49
ANISOU 40	CA PRO	6	1332	1740	2432	-218 -536 5 2 2
ATOM 41	CB PRO	6	25.571	21.722	54.847	1.000 18.21
ANISOU 41	CB PRO	6	2294	1740	2886	-224 130 434
ATOM 42	CG PRO	6	25.132	20.378	54.409	1.000 20.37
ANISOU 42	CG PRO	6	2708	2632	2399	-1078 38 - 61
ATOM 43	C PRO	6	23.576	23.091		
ANISOU 43	C PRO	6	1388	1712	55.510	1.000 14.59
ATOM 44					2443	-406 -786698
<del>-</del>		6	22.408	22.743	55.295	1.000 13.06
ANISOU 44	O PRO	6	1298	1547	2118	-283 -596 1 5
ATOM 45	N THR	7	24.048	24.326	55.313	1.000 14.56
ANISOU 45	N THR	7	1393	1678	2463	-380 -565 5 8 7
ATOM 46	CA THR	7	23.288	25.428	54.771	1.000 13.28
ANISOU 46	CA THR	7	1463	1584	1998	-469 -734 4 4 0
ATOM 47	CB THR	7	23.121	26.572	55. <b>7</b> 99	1.000 14.44
ANISOU 47	CB THR	7	1927	1652	1905	-348 -1257 3 2 9
ATOM 48	OG1 THR	7	22.454	26.102	56.998	1.000 18.44
ANISOU 48	OG1 THR	7	3136	2013	1858	-333 -829 1 7 6
ATOM 49	CG2 THR	7	22.290	27.719	55.261	1.000 14.98
ANISOU 49	CG2 THR	7	1390	1788	2513	-213 -727 4 1 2
ATOM 50	C THR	7	23.973	26.005	53.539	1.000 14.62
ANISOU 50	C THR	7	1144	2200	2212	-355 -693 7 0 4
ATOM 51	O THR	7	25.192	26.257	53.600	1.000 17.21
ANISOU 51	O THR	7	1284	2515	2738	-641 -840 9 7 5
ATOM 52	N PHE	8	23.211	26.222	52.472	1.000 12.32
ANISOU 52	N PHE	8	1165	1596	1919	-314 -534 3 7 0
ATOM 53	CA PHE	8	23.692	26.869	51.283	1.000 13.31
ANISOU 53	CA PHE	8	1554	1531	1971	-60 -295 3 4 3
ATOM 54	CB PHE	8	23.724	25.933	50.067	1.000 13.71
ANISOU 54	CB PHE	8	1479	1705	2025	-136 -232 2 3 4
ATOM 55	CG PHE	8	24.635	24.746	50.258	1.000 13.68
ANISOU 55	CG PHE	8	1225	1716		
					2257	
	CD1 PHE	8	24.147	23.503	50.628	1.000 14.10
ANISOU 56	CD1 PHE	8	1317	1710	2329	-93 231 221
ATOM 57	CD2 PHE	8	26.006	24.882	50.079	1.000 17.52
ANISOU 57	CD2 PHE	8	1239	2282	3134	-234 -56 917
ATOM 58	CE1 PHE	8	24.984	22.420	50.812	1.000 15.39
ANISOU 58	CE1 PHE	8	1473	1878	2497	-11 242 481
ATOM 59	CE2 PHE	8	26.840	23.807	50.271	
ANISOU 59	CE2 PHE	8	1179	2259	3301	-157 -143 4 2 3
ATOM 60	CZ PHE	8	26.348	22.567	50.654	1.000 17.12
ANISOU 60	CZ PHE	8	1310	2437	2757	24 - 382 978
ATOM 61	C PHE	8	22.821	28.073	50.909	
ANISOU 61	C PHE	8	1401	1513	1935	-164 -145 4 4 2

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		- 92 -	
ATOM 62 ANISOU 62	O PHE 8 O PHE 8	21.602 28.03 1392 1295	3 51.079 1.000 <u>13.18</u> 2322 -256 -400 3 6 4
ATOM 63 ANISOU 63	N SER 9	23.478 29.09	6 50.394 <u>1</u> .000 13.03
ATOM 64	N SER 9 CA SER 9	1722 1636	1593 -565 -601 4 9 0
ANISOU 64	CA SER 9 CA SER 9	22.861 30.22 1591 1468	4 49.718 1.000 12.55
ATOM 65	CB SER 9	23.743 31.47	1708 -392 -438 3 1 5 2 49.761 1.000 1 5 4 1
ANISOU 65 ATOM 66	CB SER 9	2385 1833	1637 -915 -1057 703
ATOM 66 ANISOU 66	OG SER 9 OG SER 9	23.138 32.53	9 49.007 1.000 17.99
ATOM 67	C SER 9	2504 1721 22.520 29.86	2611 -718 -999 9 2 4
ANISOU 67	C SER 9	2040 1187	2.000 12.72
ATOM 68 ANISOU 68	O SER 9 O SER 9	23.397 29.49	1606 -411 -576 4 7 6 5 47.478 1.000 16.18
ATOM 69	O SER 9 N LEU 1(	2265 2053 0 21.229 29.98	1830 -465 -38173
ANISOU 69	N LEU 1		111111111111
ATOM 70 ANISOU 70	CA LEU 1	20.798 29.71	1750 -301 -699 1 7 4 4 46.596 1.000 1 4.62
ATOM 71	CA LEU 1( CB LEU 1(		1734 -184 -784 2 2 4
ANISOU 71	CB LEU 1		3 46.436 1.000 14.72
ATOM 72	CG LEU 10	18.693 29.63	1657 -142 -657 - 168 3 45.050 1.000 14.10
ANISOU 72 ATOM 73	CG LEU 10	2087 1557	1713 -702 -695 1 4 5
ANISOU 73	CD1 LEU 10	20.21	44.582 1.000 16.23
ATOM 74	CD2 LEU 10		1595 -554 -1132 8 7 3 44.997 1.000 21.82
ANISOU 74 ATOM 75	CD2 LEU 10 C LEU 10	) 2180 2904	3206 -421 -1151 - 518
ANISOU 75	C LEU 10		45.626 1.000 15.87
ATOM 76	O LEU 10		1796 -491 -844 3 1 4 9 44.553 1.000 16.33
ANISOU 76 ATOM 77	O LEU 10	2607 1816	1780 -601 -829 2 7 6
ANISOU 77	N ALA 11 N ALA 11		45.986 1.000 17.17
ATOM 78	CA ALA 11		2115 -607 -548 1 3 9 45.129 1.000 16.56
ANISOU 78 ATOM 79	CA ALA 11	2377 1884	2029 -732 -1033 3 0 2
ANISOU 79	CB ALA 11 CB ALA 11		45.805 1.000 20.05
ATOM 80	C ALA 11		2529 -670 -674 2 5 9 44.831 1.000 16.33
ANISOU 80 ATOM 81	C ALA 11	2319 2255	1629 -754 -988 4 3 4
ANISOU 81	O ALA 11 O ALA 11	02:50,	43.677 1.000 19.66
ATOM 82	N GLU 12	3115 2559 24.558 32.085	1795 -947 -560 6 1 9 45.810 1.000 17 28
ANISOU 82 ATOM 83	N GLU 12	2686 1994	45.810 1.000 17.28 1884 -454 -1087 3 9 0
ANISOU 83	CA GLU 12 CA GLU 12		45.752 1.000 16.34
ATOM 84	CB GLU 12		1831 -474 -889 1033 47.158 1.000 16.09
ANISOU 84 ATOM 85	CB GLU 12	2440 1867	1808 -770 -820 1 0 5 8
ATOM 85 ANISOU 85	CG GLU 12 CG GLU 12		47.915 1.000 18.90
ATOM 86	CD GLU 12	2717 2127 27.115 32.657	2335 -1216 -1090 7 8 8 49.342 1.000 21 17
ANISOU 86 ATOM 87	CD GLU 12	3300 2547	49.342 1.000 21.17 2198 -1182 -1053 7 2 4
ATOM 87 ANISOU 87	OE1 GLU 12 OE1 GLU 12	27.538 31.558	49.756 1.000 22.07
88 MOTA	OE2 GLU 12	2722 3014 27.068 33.679	2650 -720 -1365 7 9 7
ANISOU 88	OE2 GLU 12	5764 2634	50.059 1.000 29.26 2722 -1279 -1848 476
ATOM 89 ANISOU 89	C GLU 12 C GLU 12	25.997 30.402	44.882 1.000 17.16
ATOM 90	C GLU 12 O GLU 12	2044 2319 26.879 30.317	2158 -624 -715 4 8 1
ANISOU 90	O GLU 12	3200 2388	44.032 1.000 18.88 1583 -1004 -306 8 9 9
ATOM 91 ANISOU 91	N LEU 13 N LEU 13	25.083 29.441	45.049 1.000 17.32
ATOM 92	N LEU 13 CA LEU 13	2176 2300 25.082 28.252	2104 -659 -386 9 4
		20.252	44.189 1.000 14.00

				- 93 -		
ANISOU 92	CA LEU	13	1734	1873	1713	-140 -170 4 9 8
ATOM 93	CB LEU	13	24.003	27.248	44.620	1.000 <del>~</del> T⊶5,.37
ANISOU 93	CB LEU	13	2205	1838	1795	-375 -149 4 6 5
ATOM 94 ANISOU 94	CG LEU	13	24.154	26.554		1.000 14.52
ATOM 95	CG LEU	13 13	1913 22.934	1803	1799	-280 -204 4 4 2
ANISOU 95	CD1 LEU	13	22.934	25.680 1817	46.193 1766	1.000 15.15 -433 185 175
ATOM 96	CD2 LEU	13	25.411	25.690	46.067	1.000 17.54
ANISOU 96	CD2 LEU	13	2119	2043	2502	-38 -419 2 7 0
ATOM 97	C LEU	13	24.876	28.626	42.725	1.000 16.54
ANISOU 97	C LEU	13	2510	2062	1710	-222 -93 565
ATOM 98	O LEU	13	25.548	28.122	41.821	1.000 18.28
ANISOU 98	O LEU	13	2685	2514	1748	-687 75 2 5 9
ATOM 99	N GLN	14	23.945	29.534	42.472	1.000 16.86
ANISOU 99 ATOM 100	N GLN CA GLN	14 14	1970 23.657	2337 30.015	2100	-557 -683 8 3 8
ANISOU 100	CA GLN	14	23.637	2404	41.132 1915	1.000 18.63 -610 -802 5 6 8
ATOM 101	CB GLN	14	22.421	30.923	41.130	1.000 19.39
ANISOU 101	CB GLN	14	3166	2176	2025	-392 -918 9 7 7
ATOM 102	CG GLN	14	21.108	30.250	41.460	1.000 19.00
ANISOU 102	CG GLN	14	2879	2383	1957	-209 -725 4 6 0
ATOM 103	CD GLN	14	19.974	31.227	41.766	1.000 18.83
ANISOU 103	CD GLN	14	3139	2118	1897	-6 -1229 4 9 4
ATOM 104 ANISOU 104	OE1 GLN OE1 GLN	14 14	20.177 3928	32.317 2407	42.314	1.000 26.10 -98 -1172 -241
ATOM 105	NE2 GLN	14	18.745	30.823	3582 41.411	-98 -1172 -241 1.000 20.94
ANISOU 105	NE2 GLN	14	2900	2716	2340	-149 -840 4 5 4
ATOM 106	C GLN	14	24.804	30.812	40.525	1.000 20.40
ANISOU 106	C GLN	14	3226	2458	2065	-795 -712 9 3 7
ATOM 107	O GLN	14	24.812	30.951	39.311	1.000 30.48
ANISOU 107	O GLN	14	5089	4340	2152	-2337 -898 1 2 1 1
ATOM 108	N GLN	15	25.734	31.309	41.329	1.000 20.35
ANISOU 108 ATOM 109	N GLN CA GLN	15 15	3252 26.909	2452 32.041	2030 40.884	-1067 -240 4 9 7
ANISOU 109	CA GLN	15	3184	3230	1901	1.000 21.88 -1152 -299 7 8 8
ATOM 110	CB GLN	15	27.288	33.100	41.920	1.000 22.20
ANISOU 110	CB GLN	15	2720	3162	2551	-1131 -770 6 9 1
ATOM 111	CG GLN	15	26.450	34.358	41.954	1.000 25.73
ANISOU 111	CG GLN	15	4496	2735	2545	-821 -233 1 2 6 9
ATOM 112	CD GLN	15	26.325	35.021	43.306	1.000 35.76
ANISOU 112	CD GLN	15	6010	3945	3631	-643 -229 -135
ATOM 113 ANISOU 113	OE1 GLN OE1 GLN	15 15	27.145 8425	34.884		1.000 49.13
ATOM 114	NE2 GLN		25.255	35.812	43/8	-2857 -2197 - 564 1.000 51.85
ANISOU 114	NE2 GLN		7190	5567	6945	62 3066 1 0 7
ATOM 115	C GLN		28.069	31.079	40.625	1.000 23.93
ANISOU 115	C GLN		3451	3513	2127	-990 145 884
ATOM 116	O GLN		29.177	31.448	40.213	1.000 28.95
ANISOU 116	O GLN		3535	4619	2845	-899 510 1225
ATOM 117	N GLY		27.828	29.794	40.891	1.000 25.86
ANISOU 117 ATOM 118	N GLY CA GLY		4089	3282	2457	-889 -36 469
ANISOU 118	CA GLI		28.812 4785	28.763 3562	40.649 2671	1.000 29.00 -677 765 255
ATOM 119	C GLY		29.741	28.546	41.814	
ANISOU 119	C GLY		3427	3490	2754	-264 1422 6 7 3
ATOM 120	O GLY		30.805	27.955	41.625	1.000 29.63
ANISOU 120	O GLY		3925	3267	4068	-66 1997 5 2 3
ATOM 121	N LEU		29.387	28.979	43.015	1.000 22.50
ANISOU 121	N LEU		3266	2713	2569	-39 923 733
ATOM 122	CA LEU		30.234	28.727		1.000 21.73
ANISOU 122	CA LEU	17	2299	2931	3025	-282 867 748

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ANISOU 184 NH2 ATOM 185 C ANISOU 185 C ANISOU 186 O ANISOU 187 N ANISOU 187 N ANISOU 188 CA ANISOU 188 CA ANISOU 189 CB ANISOU 190 CG ANISOU 191 CD ANISOU 191 CD ANISOU 192 NE ANISOU 192 NE ANISOU 193 CZ ANISOU 193 CZ ANISOU 194 NH1 ANISOU 194 NH1 ANISOU 195 NH2 ANISOU 195 NH2 ANISOU 196 C ANISOU 197 O ANISOU 196 C ANISOU 197 O ANISOU 197 O ANISOU 198 N ANISOU 199 CA ANISOU 200 CB ANISOU 201 SG ANISOU 201 SG ANISOU 202 C ANISOU 203 O ANISOU 204 N	2 ARG 23 ARG 224 ARG 224 ARG 224 ARG 224 ARG 224 ARG 224 ARG ARG 224 ARG ARG 224 ARG ARG 224 ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	2261 28.045 1071 27.335 1443 28.952 1024 29.193 1443 30.466 1244 31.787 1438 32.979 1163 33.636 5800 33.973 4738 33.731 2650 34.579 5339 27.972 1549 27.536 1706 27.355 907 1824 26.105 942 1838 25.660 1150 23.973 1465 25.660 1150 23.973 1465 25.001 893 1897 24.360 1347 24.798	20.114 5328 16.713 2061 15.687 2244 16.988 2156 16.003 2589 16.422 3486 16.217 5078 16.537 5831 17.804 7316 18.776 18.776 18.779 18.779 18.87 14.779 18.90 17.011 17.040 17.011 17.040 17.011 17.040 17.011 17.040 17.011 17.040 17.011 17.040 17.011 17.040 18.491 17.59 18.580 15.377 1426 16.461	6121 46.420 2589 46.410 2497 47.353 2623 48.430 2693 49.148 3289 48.57 49.36 49.37 49.37 49.448 49.33 49.448	-562 77 86 1.000 15.06 167 -32 -234 1.000 16.28 -118 -71 -277 1.000 15.27 -52 -21 2 9 1.000 17.70 275 -2 2 1 5 1.000 21.11 484 -257 3 8 4 1.000 30.46 426 441 3 0 8 1.000 33.50 208 370 4 5 8 1.000 51.46 -2596 -1688 1 1 6 5 1.000 46.72 -1719 -1822 1 3 1 6 1.000 42.82 513 -991 1 2 1 6 1.000 17.16 129 140 2 9 5 1.000 15.38 72 -388 1 0 4 1.000 12.91 4 -386 1 5 1 1.000 12.45 8 -480 8 1 1.000 12.45 8 -480 8 1 1.000 14.90 -164 -26 - 1 8 1.000 11.67 -136 -604 1 8 4 1.000 14.90 -164 -26 - 1 8 1.000 11.67 3 -64 - 86 1.000 12.73 -233 -196 1 2 3 1.000 11.70
ANISOU 196 C	ARG 24	1549	2071	2900	1.000 17.16
ANISOU 197 O	ARG 24			49.713	1.000 15.38
		27.355	17.011	49.696	1.000 12.91
ATOM 199 CA	CYS 25			76 -25	4 - 386 151
7.000	-	942 1838	, TA	49 -17	8 -480 8 1
ANISOU 200 CB	CYS 25	1150	18.491		1.000 11.67
ANISOU 201 SG		23.973 1465		51.425	1.000 14.90
ATOM 202 C	CYS 25	25.001	16.225	49.769	-164 -26 - 18 1.000 11.67
ATOM 203 O	CYS 25			45 -28	3 -64 - 86
ATOM 204 N		1347	1426	2064	-233 -196123
ANISOU 204 N	LEU 26	1102	1530	48.470 1814	1.000 11.70 -128 -390 1
ANISOU 205 CA	LEU 26 LEU 26	23.766 1190	15.716 1476	47.735	1.000 11.11
	LEU 26 LEU 26	23.674 1345	16.198	46.285	-238 -79 -194 1.00011.54
ATOM 207 CG	LEU 26	23.242	1522 17.638		-75 -84 -202 1.000 12.42
ATOM 208 CD1			1542 17.993	1978	-153 -167 - 40
ANISOU 208 CD1 ATOM 209 CD2	LEU 26 LEU 26	1428	1916	2270	1.000 14.77 43 131 4 0 1
ANISOU 209 CD2	LEU 26	1384	17.885 2061	2047	1.000 14.45 264 -32 3 2 1
ANISOU 210 C	LEU 26 LEU 26		14.209 1542	47.780	1.000 12.93
	LEU 26 LEU 26	23.011	13.461	48.008	1.000 13.78
ATOM 212 N	ARG 27	25.196	1450 13.721	47.576	-305 -426 - 51 1.000 14.09
ATOM 213 CA	ARG 27 ARG 27		1729 12.283	2108	151 -530 - 105
3 m o 3 (	ARG 27 ARG 27	2260	1690	1897	1.000 15.39 186 141 -354
•		20.040	12.122	46.900	1.000 17.04

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ANISOU	214	C3	ARG	27	2259	2356	1861	517 49 - 248
ATOM	215	ĊĠ	ARG		27.502			1.000 2-5 - 08
					3110			
ANISOU		CG	ARG	27			3583	1105 606 - 399
MOTA	216	CD	ARG	27	28.995			1.000 30.32
ANISOU	216	CD	ARG	27	2976	3836	4710	1190 720 -1381
ATOM	217	NΞ	ARG	27	29.818		47.581	1.000 36.51
ANISOU		NE	ARG	27	3633	4937	5301	121 391 -1429
MOTA	218	CZ	ARG	27	30.988		47.560	1.000 38.07
ANISOU	218	CZ	ARG	27	3334	5192	5941	364 661 -1776
ATOM	219	NH1	ARG	27	31.565	12.340	46.401	1.000 48.56
ANISOU		NH1	ARG	27	4482	7688	6280	-1305 736 -1326
	220	NH2		27	31.606	12.328	48.701	
ATOM								1.000 40.23
ANISOU		NH2		27	2891	6127	6266	457 717 - 2463
MOTA	221	С	ARG	27	25.479	11.630	48.949	1.000 14.66
ANISOU	221	С	ARG	27	1720	1617	2233	135 -33 - 42
ATOM	222	0	ARG	27	24.968	10.499	49.072	1.000 17.44
ANISOU		Ö	ARG	27	1981	1533	3114	98 - 394 155
MOTA	223	N	ASP	28	26.031	12.308	49.973	1.000 13.72
ANISOU	223	И	ASP	28	1703	1366	2146	317 -327 3 1 9
ATOM	224	CA	ASP	28	26.227	11.701	51.277	1.000 15.33
ANISOU		CA	ASP	28	1886	1704	2234	538 -247 3 9 1
ATOM	225	CB	ASP	28	27.541	12.280	51.842	1.000 18.31
ANISOU		CB	ASP	28	2092	2709	2155	186 -465 5 4 4
ATOM	226	CG	ASP	28	28.785	11.875	51.083	1.000 23.06
ANISOU	226	CG	ASP	28	2002	3583	3176	-96 -50 478
ATOM	227		ASP	28	28.741	10.904	50.290	1.000 25.09
ANISOU			ASP	28	2515	2855	4163	830 406 440
MOTA	228		ASP	28	29.831	12.528	51.283	1.000 30.05
ANISOU		OD2	ASP	28	1919	4262	5236	-216 -695 1 0 5 8
MOTA	229	С	ASP	28	25.092	11.910	52.267	1.000 14.90
ANISOU		С	ASP	28	2071	1435	2154	411 -203 2 1 7
ATOM	230	Ö	ASP	28	24.967	11.093	53.200	1.000 14.50
ANISOU		0	ASP	28	1878	1501	2132	444 -265 1 7 9
$\mathtt{MOTA}$	231	N	LYS	29	24.317	12.975	52.096	1.000 12.90
ANISOU	231	N	LYS	29	1487	1290	2126	77 -276 136
ATOM	232	CA	LYS	29	23.265	13.368	53.029	1.000 12.95
ANISOU		CA	LYS	29	1369	1649	1904	8 -390 1 4
								1.000 12.71
MOTA	233	CB	LYS	29	23.699	14.653	53.763	
ANISOU		CB	LYS	29	1105	1581	2145	209 -359 - 30
ATOM	234	CG	LYS	29	25.016	14.504	54.518	1.000 16.11
ANISOU	234	CG	LYS	29	1413	1998	2711 .	21 -818 -161
ATOM	235	CD	LYS	29	25.449	15.727	55.309	1.000 18.24
ANISOU		CD	LYS	29	2500	1989	2442	-47 -1140 - 14
								1 000 10 36
MOTA	236	CE	LYS	29	26.789	15.445	56.002	1.000 19.36
ANISOU	236	CE	LYS	29	2038	3171	2148	-90 -822 - 725
ATOM	237	ΝZ	LYS	29	27.515	16.696	56.351	1.000 26.61
ANISOU		ΝZ	LYS	29	2592	3146	4373	-309 -1571 -353
ATOM	238	C	LYS	29	21.888	13.550	52.386	1.000 11.62
ANISOU		С	LYS	29	1432	1153	1831	52 - 290 2 4
MOTA	239	0	LYS	29	20.877	13.028	52.880	1.000 12.57
ANISOU	239	0	LYS	29	1426	1556	1792	-97 -282 1 0 0
ATOM	240	N	GLY	30	21.779	14.280	51.284	
ANISOU		N	GLY	30	1359	1454	1741	-5 -310 7 8
ATOM	241	CA	GLY	30	20.510	14.478	50.562	
ANISOU		CA	GLY	30	1192	1497	1465	-158 -116 - 18
ATOM	242	С	GLY	30	19.544	15.433	51.242	1.000 11.15
ANISOU	1 242	С	GLY	30	1137	1143	1955	-260 -154 - 131
ATOM	243	Ö	GLY	30	18.337	15.374	50.963	
						1082		
ANISOU		0	GLY	30	1247		1949	-56 -419 1 0 4
ATOM	244	N	LEU	31	20.064	16.278		
DORINA	J 244	N	LEU	31	1292	894 18	321 -9	98 -367 8 9

- 98 -ATOM 245 CA LEU 17.324 52.803 1.000 11.07 31 19.272 ANISOU 245 CA LEU 31 1345 1111 1752 46 -528 - 3 3 MOTA 246 CB LEU 16.777 53.975 1.000 14.44 31 18.465 ANISOU 246 CB LEU 31 1753 1671 2062 -284 -80 -178 MOTA 247 CG LEU 31 19.113 16.629 55.333 1.000 17.74 ANISOU 247 CG LEU 31 2456 2220 2064 -172 -115 4 9 9 MOTA 248 CD1 LEU 31 15.978 56.371 1.000 26.19 18.220 ANISOU 248 CD1 LEU 31 2716 4691 2543 -1224 -213 1016 ATOM 249 CD2 LEU 31 20.388 15.821 55.182 1.000 22.77 ANISOU 249 CD2 LEU 31 3121 2633 2899 650 -18 1487 MOTA 250 C LEU 31 18.498 53.195 1.000 10.95 20.176 ANISOU 250 С LEU 31 1041 1129 1989 180 -318 - 223 MOTA 251 0 LEU 18.314 53.424 1.000 10.89 31 21.376 ANISOU 251 0 LEU 1015 31 1171 1952 69 -160 204 ATOM 252 Ν PHE 32 19.570 19.688 53.219 1.000 11.42 ANISOU 252 PHE 32 1134 995 2211 75 -273 6 5 ATOM 253 CAPHE 32 20.916 53.545 1.000 10.33 20.280 ANISOU 253 CA PHE 32 1071 1152 1703 -57 -288 - 33 254 ATOM CВ PHE 32 21.244 21.307 52.422 1.000 12.25 ANISOU 254 CB PHE 32 1054 1729 1872 -113 -173 - 5 ATOM 255 CG PHE 32 20.624 21.346 51.041 1.000 11.94 ANISOU 255 CG PHE 32 1158 1572 1809 -281 -148 1 2 2 ATOM 256 CD1 PHE 32 20.522 20.188 50.270 1.000 11.12 ANISOU 256 CD1 PHE 32 1070 1308 1846 -182 -458 3 1 8 MOTA 257 CD2 PHE 32 20.145 22.528 50.513 1.000 12.14 ANISOU 257 CD2 PHE 32 1618 1353 1639 -300 -185 - 47ATOM 258 CE1 PHE 32 19.943 20.212 49.015 1.000 12.00 ANISOU 258 CE1 PHE 32 1342 1377 1840 -301 -468 3 3 2 MOTA 259 CE2 PHE 32 22.534 49.266 1.000 12.79 19.553 ANISOU 259 CE2 PHE 32 1858 1543 1457 -86 -34 2 8 MOTA 260 CZ PHE 32 19.416 21.376 48.503 1.000 11.50 ANISOU 260 -CZ PHE 32 1623 1414 1331 -76 -272 2 1 7 MOTA 261 С PHE 32 19.310 22.071 53.762 1.000 9.82 ANISOU 261 C PHE 32 1015 1042 1674 -120 -367 - 77 MOTA 262 0 PHE 32 18.165 21.990 53.285 1.000 11.29 ANISOU 262 0 PHE 32 1097 1286 1906 -95 -495 - 77 ATOM 263 N TYR 19.736 23.099 33 54.493 1.000 12.68 ANISOU 263 N TYR 33 1606 1053 2158 -57 -766 - 159 ATOM 264 CA TYR 33 18.945 24.335 54.607 1.000 10.64 ANISOU 264 CATYR 33 1491 1173 1380 -77 -97 -132 ATOM 265 CBTYR 33 19.141 25.022 55.955 1.000 10.85 ANISOU 265 CBTYR 1019 33 1725 1379 -260 -224 - 164 MOTA 266 CG TYR 33 18.545 24.331 57.156 1.000 10.71 ANISOU 266 CG TYR 33 1173 1552 1342 -45 -230 - 117MOTA 267 CD1 TYR 33 17.266 24.643 57.619 1.000 11.64 ANISOU 267 CD1 TYR 33 1385 1441 1596 -68 83 - 94 MOTA 268 CE1 TYR 16.694 24.023 58.719 1.000 13.60 33 ANISOU 268 CE1 TYR 33 1879 1483 -147 339 - 26 1804 MOTA 269 CD2 TYR 33 23.364 57.853 1.000 14.04 19.273 ANISOU 269 CD2 TYR 33 1604 2040 1689 132 -509 1 2 7 ATOM 270 CE2 TYR 18.711 22.752 58.964 1.000 15.75 33 ANISOU 270 CE2 TYR 33 1872 2227 1886 -187 -701 4 3 3 MOTA 271 CZTYR 33 17.438 23.078 59.387 1.000 16.02 ANISOU 271 CZTYR 33 2205 1939 1942 -332 -154 3 0 0 ATOM 272 OH TYR 33 16.919 22.454 60.504 1.000 19.95 ANISOU 272 OH TYR 33 3412 2154 2015 -60 278 400 MOTA 273 С 25.253 53.452 1.000 10.92 TYR 19.357 33 ANISOU 273 C 33 TYR 1249 1448 1453 -125 -271 1 4 9 ATOM 274 0 TYR 33 20.514 25.192 53.006 1.000 11.50 ANISOU 274 0 TYR 33 1204 1375 1791 -98 -270 2 8 1 MOTA 275 N LEU 34 18.399 26.049 53.000 1.000 11.28



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ANISOU	275	N	LEU	3 4	1159	1265		-210 -149 1 2 1
MOTA	276			34			51.864	1.000 <del>-12</del> , 99
ANISOU	276	C.A.	LEU		1565	1444		81 -478 274
ATOM	277		LEU	34	17.757	26.420	50.682	1.000 13.96
ANISOU			LEU	3 4	2007	1301	1995	-430 -459 3 2 1
ATOM	278		LEU	3 4	17.990	27.112	49.334	1.000 13.81
ANISOU			LEU		2085	1322	1839	-331 -365 1 9 8
ATOM	279	CD1			19.308	26.691	48.704	1.000 15.94
ANISOU		CD1		34	2123	1793	2140	-10 -313 6 0 7
ATOM	280	CD2		34	16.818	26.799	48.411	1.000 16.36
ANISOU		CD2		34	2186	1837	2193	122 -721 1 3 4
MOTA	281	С	LEU	34	18.195	28.361	52.241	1.000 13.03
ANISOU		С	LEU	34	1676	1418	1857	31 -643 218
ATOM	282	0	LEU	34	17.055	28.647	52.595	1.000 13.99
ANISOU	282	0	LEU	34	1690	1281	2344	140 -714 8 5
ATOM	283	N	THR	35	19.148	29.283	52.175	1.000 15.03
ANISOU	283	N	THR	35	1837	1584	2288	-118 -625 - 3
ATOM	284	CA	THR	3 5	18.918	30.704	52.369	1.000 14.80
ANISOU	284	CA	THR	3 5	1866	1560	2196	-169 -175 -144
MOTA	285	CB	THR	35	20.013	31.366	53.232	1.000 15.65
ANISOU	285	CB	$\mathtt{THR}$	3 5	2025	1719	2202	-149 -204 - 281
ATOM	286	OG1	THR	3 5	21.276	31.115	52.601	1.000 18.81
ANISOU			THR	3 5	1885	2679	2583	-279 -229 - 728
MOTA	287		$\mathtt{THR}$	3 5	20.138	30.811	54.622	1.000 18.84
ANISOU		CG2		3 5	2523	2207	2427	-850 -510 1 5 5
MOTA	288	С	THR	3 5	18.915	31.456	51.043	1.000 15.07
ANISOU		C	THR	35	1904	1473	2348	-57 -283 - 70
ATOM	289	0	THR	35	19.209	30.909	49.973	
ANISOU		0	THR	35	2034	1520	2145	-215 -372 8 9 1.000 17.46
ATOM	290	N	ASP	36	18.564	32.739	51.086 2968	-209 -766 - 120
ANISOU		N	ASP	36	2302	1366	49.924	
ATOM	291	CA	ASP	36	18.618	33.606 1592	3063	112 -660 8 6
ANISOU		CA CB	ASP	36 36	2150 20.063	33.845	49.471	1.000 17.91
ATOM	292		ASP	36	2153	1584	3067	84 -587 - 42
ANISOU	293	CB CG	ASP ASP	36	20.948	34.545	50.469	1.000 19.23
ATOM ANISOU		CG	ASP	36	2575	2160	2571	-642 -324 1 8 1
ANISOC	294		ASP	36	20.426	35.304		1.000 24.17
ANISOU			ASP	36	2843	3055	3284	152 -1013 -652
MOTA	295		ASP	36	22.199	34.355		
ANISOU			ASP	36	2637	2571	2772	-382 -834 - 393
ATOM	296	C	ASP	36	17.783	33.038		1.000 18.20
ANISO		Č	ASP	36	2402	1736	2779	-446 -390 1 9 1
ATOM	297	Õ	ASP	36	18.222	33.063	47.629	1.000 18.98
ANISO		Ō	ASP	36	2127	2022	3062	-464 <b>-</b> 60 <b>-</b> 252
ATOM	298	N	CYS	37	16.593	32.547	49.077	1.000 17.22
ANISO		N	CYS	37	1873	2190	2479	63 -350 - 1
MOTA	299	CA	CYS	37	15.730	31.945	48.043	1.000 15.98
ANISO		CA	CYS	37	1997	1590	2485	-81 -65 -184
ATOM	300	CB	CYS	37	15.621	30.423		
ANISO	U 300	CB	CYS	37	2112	1790	3268	-114 -405 5 7 0
ATOM	301	SG	CYS	37	14.753	29.917	49.759	
ANISO	U 301	SG	CYS	37	2532	1683	3164	-74 -230 3 2 2
ATOM	302	С	CYS	37	14.349		47.958	
ANISO		С	CYS	37	1992	1669	2465	-175 -504 1 6
ATOM	303	0	CYS		13.483			
ANISO	U 303	0	CYS		2761	1769	3296	-241 -1333 5 1
MOTA	304		GLY					
ANISO			GLY			1572	3381	209 -898 - 111
ATOM	305							
ANISC	ช 305	CA	. GLY	38	1608	2126	3164	141 -999 - 6

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ATOM	306	C	GLY	38	11.843	33.86	4 40 504	
ANISC	DU 306		GLY			2574		
ATOM	307		GLY		10.677	34.27	3180	262 <del>-9</del> 7 - 455
ANISC			GLY			3027		1.000 22.75
ATOM	308	N	LEU		12.241	32.982	3073	241 79 - 9 7
ANISC			LEU		2112	3318		
ATOM	309		LEU		11.443	32.357	2903	-65 -102 -154
ANISO					3141	3610		1.000 26.16
ATOM	310				11.220	30.868	3188	-1071 162 -400
ANISO		CВ	LEU		2980	3192		1.000 28.13
ATOM	311	CG	LEU		10.296	30.434	4516	-352 -848 2 5 8
ANISO		CG	LEU	39	3352	2591		1.000 27.39
ATOM	312	CD:	1 LEU	39	10.472	28.940	4463	541 -637 -1052
ANISO		CD:	l LEU	39	3375	2293	49.910 5221	1.000 28.66
ATOM	313	CD2	FEU S	39	8.838	30.768	50.478	581 -150 - 190
ANISO		CD2	2 LEU	39	3155	2985	5496	
ATOM	314	С	LEU	39	12.060	32.430	52.949	1275 -1485 -208
ANISO		C	LEU	39	2868	3969	3143	1.000 26.26
ATOM	315	0	LEU	39	13.105	31.861	53.256	
ANISO		0	LEU	39	4990	4057	4470	1.000 35.57
ATOM	316	N	$\mathtt{THR}$	40	11.388	33.136	53.827	
ANISOU ATOM		N	THR	40	3425	3883	2803	
ANISOU	317	CA	THR	40	11.676	33.329	55.228	-703 -191 1 0 2 1.000 22.95
ATOM		CA	THR	40	1972	3864	2886	4 -608 518
ANISOU	318	C	THR	40	10.380	33.424	56.031	4 -608 518 1.000 27.03
ATOM		C	THR	40	2331	4900	3040	-690 -220 - 3
ANISOU	319	0	THR	40	9.254	33.316	55.537	1.000 25.98
ATOM	320	0	THR	40	2148	4860	2864	-546 36 - 720
ANISOU	320	CB	THR	40	12.476	34.624	55.456	1.000 27.16
ATOM	321	CB	THR	40	2646	4799	2874	-932 -391 1 4 8
ANISOU		061	THR	40	11.639	35.687	54.986	1.000 36.24
ATOM	322	CC3	THR	40	5158	3872	4740	-472 -136 6 6 0
ANISOU	1 322	CG2	THR	40	13.771	34.669	54.659	1.000 34.29
ATOM	323	N CG2	THR	40	5268	3289	4470	-1303 2206 4 2 9
ANISOU	323	N	ASP	41	10.524	33.635	_	1.000 28.20
ATOM	324	CA	ASP ASP	41	2270	5223	3223	-711 -317 - 479
ANISOU	324	CA	ASP	41	9.324	33.604	58.191	1.000 25.10
ATOM	325	C	ASP	41	1935	4633	2968	13 -551 -505
ANISOU	325	Ċ	ASP	41	8.418	34.785	57.896	1.000 24.69
ATOM	326	Õ	ASP	41 41	2686	3839	2855	-446 -749 - 241
ANISOU	326	Ö	ASP	41	7.219	34.846	58.163	1.000 24.79
ATOM	327	ČВ			2757 9.728	2721	3941	174 -584 - 141
ANISOU	327	CB	ASP	41	2221		59.678	1.000 28.21
MOTA	328	ĊĠ	ASP	41	9.892	5503	2995	892 -594 - 555
ANISOU	328	ĊĠ	ASP	41	6437	32.129	60.180	1.000 42.46
MOTA	329	OD1	ASP	41	9.705	5911	3784	-1196 -1257 8 2 6
ANISOU	329	OD1	ASP	41	12184	31.161	59.401	1.000 55.96
ATOM	330	OD2	ASP	41	10.214	5138	3940	-2654 -82 1249
ANISOU	330	OD2	ASP	41	10370	31.951	61.383	1.000 61.55
ATOM	331	N	THR	42	8.991	7470	5548	-4396 -4720 2309
ANISOU	331	N	THR	42	3761	35.807	57.305	1.000 29.30
MOTA	332	CA	THR	42	8.255	4531	2839	-1404 -1089 - 72
ANISOU	332	CA	THR	42	4852	36.976 3472	56.863	1.000 33.69
MOTA	333	С	THR		7.199	36.598	4475	-1524 -819 - 127
ANISOU		С	THR		3354	30.598	55.834	1.000 29.14
ATOM	334	0	THR		6.026	36.969	4667	204 -648 - 277
ANISOU		0	THR		3578	2980		1.000 36.90
ATOM	335		THR		9.282	37.967		603 -176 6 4 3
ANISOU		CB	THR		5831	4318		1.000 40.80
ATOM	336	OG1	THR		10.288	38.317	5354	-2254 -450 3 7
					_ 3 0	-0.51/	57.263	1.000 46.30

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ANISOU 336 ATOM 337 ANISOU 337 ANISOU 338 ANISOU 338 ATOM 339 ANISOU 340 ANISOU 340 ANISOU 341 ANISOU 341 ANISOU 341 ANISOU 342 ANISOU 342 ANISOU 343 ANISOU 343 ANISOU 344 ANISOU 344 ANISOU 345 ANISOU 345 ANISOU 346 ANISOU 346 ANISOU 346 ANISOU 346 ANISOU 347 ANISOU 346 ANISOU 347 ANISOU 347 ANISOU 347 ANISOU 347 ANISOU 347 ANISOU 348 ANISOU 349 ANISOU 350 ANISOU 351 ANISOU 351 ANISOU 351 ANISOU 352 ANISOU 353 ANISOU 353 ANISOU 353 ANISOU 353 ANISOU 355 ANISOU 357 ANISOU 357 ANISOU 358 ANISOU 359	C ALA 45 O ALA 45 O ALA 45 CB ALA 45 CB ALA 45 N SER 46	2508 5.117 4009 5.978 5094 5.284 5971 4.485 7665 6.302 7096 4.000 3835 2.913 4402 4.238 2897 3.382 2716 1.943 2697 1.021 2762 3.975 3.259 1.729	3682 39733387734360 35.3554683 34.324 33973824.329738294.138 34.5324.5324.5324.5329736.05427 35.764736.0764736	4319 53.810 3913 54.330 4363 53.764 7717 52.608 3779 52.010 5377 52.826 5145 53.880 4627 52.433 8050 55.426 3964 55.959 4187 56.727 3448 57.533 3398 56.656 4514 58.361 4080 56.841 4800 56.867 3768 57.547 58.623 4761 58.361 58.361 58.361 58.361 58.361 58.361 56.867 57.547 58.361 58	-3163 -1173 1 7 7 1.000-15.59 -2166 -1048 2 3 8 1.000 31.74 -673 -223 - 7 8 2 1.000 35.40 -1510 -860 3 2 9 1.000 28.03 -41 -919 1 6 8 1.000 38.18 -66 -2774 1 4 6 9 1.000 38.89 -2546 -860 - 3 9 3 1.000 45.47 -2936 -92 - 2 8 9 1.000 46.40 -3155 548 - 1 2 1 0 1.000 55.20 -2062 -1002 - 6 6 9 1.000 56.77 -2652 939 - 1 2 5 8 1.000 22.72 464 -476 - 4 5 0 1.000 56.76 140 570 - 9 8 6 1.000 28.25 -153 277 - 5 6 2 1.000 37.95 -1148 2039 - 1 4 0 3 1.000 36.97 1150 2171 1 8 6 1.000 37.95 -1148 2039 - 1 4 0 3 1.000 36.97 1150 2171 1 8 6 1.000 37.95 -1148 2039 - 1 4 0 3 1.000 36.97 1150 2171 1 8 6 1.000 37.95 -1148 2039 - 1 4 0 3 1.000 36.97 1150 2171 1 8 6 1.000 37.95 -1148 2039 - 1 4 0 3 1.000 36.97 1150 2171 1 8 6 1.000 37.95 -784 709 - 1 2 5 7 1.000 28.74 -562 710 - 2 0 6 1 1.000 24.95 -784 709 - 1 2 5 7 1.000 22.50 -565 560 - 1 1 4 6 1.000 36.30 -1912 1332 - 3 4 0 4 1.000 26.85
ATOM 356 ANISOU 356 ATOM 357 ANISOU 357 ATOM 358 ANISOU 358	CA ALA 45 CA ALA 45 C ALA 45 C ALA 45 O ALA 45 O ALA 45	3.382 2716 1.943 2697 1.021 2762	34.751 2817 35.014 3110 34.515	58.623 4761 58.195 3673 58.875	1.000 27.09 -751 467 -2140 1.000 24.95 -784 709 -1257 1.000 22.50
ANISOU 359	CB ALA 45 N SER 46 N SER 46 CA SER 46 CA SER 46 CB SER 46 CB SER 46 OG SER 46 OG SER 46 C SER 46 C SER 46	3259 1.729 3258 0.380 3686 0.422 5428 0.630 7730 -0.408 2797	4219 35.779 3756 36.052 3189 36.950 3467 38.289 3349 34.787 2469	6315 57.128 3187 56.642 2611 55.392 3395 55.772 6313 56.307 2572	-1912 1332 - 3404 1.000 26.85 -1732 618 - 1184 1.000 24.97 -1223 511 - 1105 1.000 32.35 -2232 70 - 458 1.000 45.77 -2746 2499 - 807 1.000 20.63 -423 -151 - 542
ANISOU 365 ATOM 366 ANISOU 366	O SER 46 O SER 46 N ALA 47 N ALA 47	-1.578 3120 0.211 3096	34.672 2486 33.855 2167	56.698 2725 55.590 3244	1.000 21.93 -559 305 -403 1.000 22.39 -488 394 -368

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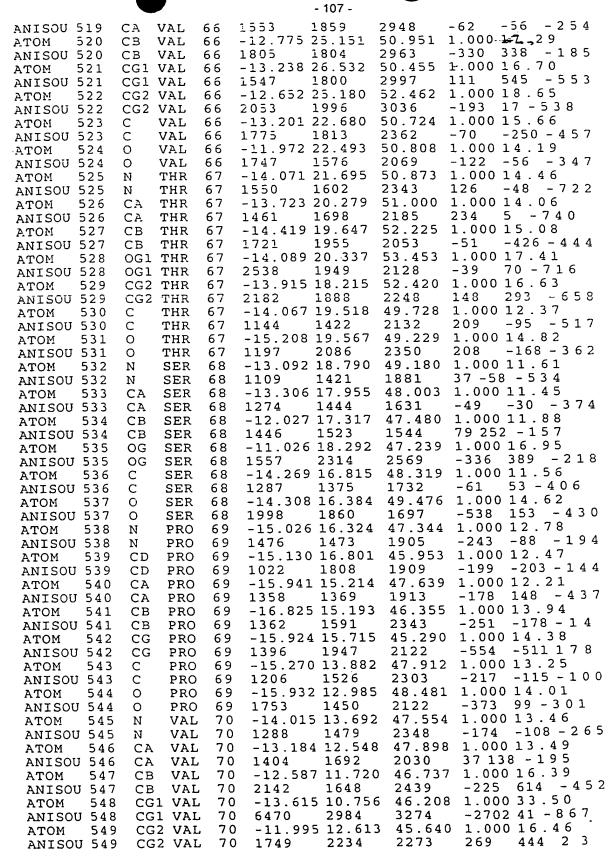
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ATOM	367	C.A.	ALA	47	-0.397	32.596	55.176	1.000 19.54
ANISOU		CA	ALA	47	2746	1863	2814	-289 362 - 18
ATOM ANISOU	368	CB	ALA	47	0.548	31.900	54.191	1.000 23.54
ATOM	369	СВ	ALA	47	3524	1717	3705	-617 1237 - 159
ANISOU		C	ALA	47	-0.715	31.714	56.381	1.000 19.95
ATOM	370	C O	ALA	47	2282	2546	2752	-327 19 2 5 7
ANISOU		0	ALA	47	-1.836	31.199	56.518	1.000 19.66
ATOM	371	И	ALA LYS	47	2489	2589	2393	-614 211 -165
ANISOU	_	N	LYS	48 48	0.270 2713	31.558	57.268	1.000 18.24
ATOM	372	C.A.	LYS	48	0.042	1966	2253	-210 -139 - 912
ANISOU	372	CA	LYS	48	2398	30.782 2625	58.486	1.000 19.33
MOTA	373	С	LYS	48	-1.110	31.329	2321 59.322	43 -312 -563
ANISOU		С	LYS	48	2476	2556	2785	1.000 20.57
ATOM	374	0	LYS	48	-2.022	30.613	59.771	-326 83 - 566
ANISOU		0	LYS	48	3207	2598	1923	1.000 20.34 -521 139 -340
ATOM	375	CB	LYS	48	1.352	30.758	59.294	1.000 24.61
ANISOU	_	CB	LYS	48	2400	3792	3158	-258 -556 - 80
ATOM	376	CG	LYS		1.237	29.873	60.531	1.000 30.84
ANISOU ATOM		CG	LYS	48	4306	4044	3366	-291 -1504 277
ANISOU	377	CD	LYS	48	1.837	30.575	61.736	1.000 41.45
ATOM	378	CD CE	LYS	48	6742	5755	3251	-1067 -1382 - 356
ANISOU		CE	LYS LYS	48	1.625	29.717	62.966	1.000 41.63
ATOM	379	NZ	LYS	48 48	6620	6124	3073	-466 -1047 -353
ANISOU		NZ	LYS	48	1.074 5883	30.497	64.112	1.000 42.62
ATOM	380	N	ASP	49	-1.110	6866 32.625	3444	460 -1193 - 425
ANISOU		N	ASP	49	2348	2602	59.607	1.000 19.18
MOTA	381	CA	ASP	49	-2.127	33.243	2337 60.433	-464 100 -806
ANISOU	381	CA	ASP	49	2555	2986	2801	1.000 21.95 -791 617 -1035
MOTA		CB	ASP	49	-1.868	34.756	60.611	-791 617 -1035 1.000 23.97
ANISOU		CB	ASP	49	2827	2872	3409	-250 -79 -1325
ATOM	383	CG	ASP	49	-0.681	35.078	61.492	1.000 25 . 41
ANISOU		CG	ASP	49	2787	3405	3464	-365 113 -1866
ATOM	384	OD1		49	-0.153	34.153	62.143	1.000 30.75
ANISOU ATOM	384		ASP	49	3572	4181.	3932	-254 -967 -1667
ANISOU		OD2	ASP	49	-0.235	36.256	61.563	1.000 30.78
ATOM	386	C C	ASP	49	3303	3649	4742	-710 344 -2413
ANISOU	386	C	ASP	49 49	-3.543	33.061	59.904	1.000 21.44
ATOM	387	Ö	ASP	49	2465 -4.476	2651	3030	-388 540 -900
ANISOU		ŏ	ASP	49	2346	32.770 2181	60.654	1.000 20.72
ATOM		N	LEU	50	-3.731	33.269	3347 58.596	-279 550 -726
NOSINA	388	N	LEU	50	2942	2712	3191	1.000 23.28
MOTA	389	CA	LEU	50	-5.086	33.185	58.068	-1251 216 -644
ANISOU		CA	LEU	50	3104	1796	3815	1.000 22.94 -575 -205 -1079
ATOM	390	CB	LEU	50	-5.204	33.861	56.696	1.000 28.78
ANISOU		CB	LEU	50	3948	2453	4535	-852 -755 - 254
ATOM	391	CG	LEU	50	-6.620	34.246	56.260	1.000 25.30
ANISOU ATOM		CG	LEU	50	3800	2294	3520	30 325 - 5 3 1
ANISOU	392	CD1		50	-7.552	34.478	57.441	1.000 44.77
ATOM		CD1		50	6382	4432	6196	-475 3026 - 1060
ANISOU	393 393	CD2		50	-6.625	35.485	55.385	1.000 32.52
ATOM	394	CD2		50	5861	1962	4533	752 354 - 433
ANISOU	394	C	LEU LEU	50	-5.566	31.737	57.982	1.000 21.12
ATOM	395	0	LEU	50 50	2559	1870	3595	-643 742 -1270
ANISOU		0	LEU	50	-6.772 2491	31.494	58.175	1.000 21.13
ATOM	396	N	VAL	51	-4.681	2457	3083	-543 579 -1097
ANISOU		N	VAL	51	2517	30.769	57.715	1.000 16.27
ATOM	397	CA	VAL	51	-5.186	1843 29.370	1823	-302 -3 -646
					100	29.3/0	57.701	1.000 18.07

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ANISOU	397	CA	VAL	51	3154	1763	1947	-401 -15 -427
	398	CB	VAL	51	-4.281	28.415	56.889	1.000 1 6.007
ANISOU	398	CB	VAL	51	2981	1629	1496	-621 -255 - 501
	399	CG1		51	-3.002	28.114	57.668	1.000 18.99
ANISOU		CG1		51	2959	2382	1875	-383 -100 3 0 2
MOTA	400	CG2		51	-5.006	27.119	56.497	1.000 22.16
ANISOU		CG2		51	4569	2121	1728	-1393 64 - 869
ATOM	401	C	VAL	51	-5.446	28.899	59.114	1.000 17.74
ANISOU	401	C 0	VAL	51 51	2508	2223	2009	-435 142 -445
ATOM ANISOU		0	VAL VAL	51	-6.430 3005	28.187 2160	59.346 2345	1.000 19.76 -692 726 -1021
ANISOU	403	N	ILE	52	-4.671	29.263	60.125	1.000 20.23
ANISOU		N	ILE	52	2980	2945	1760	-649 364 -902
ATOM	404	CA	ILE	52	-4.990	28.875	61.507	1.000 20.17
ANISOU		CA	ILE	52	3200	2665	1800	-758 627 -1134
ATOM	405	CB	ILE	52	-3.847	29.230	62.469	1.000 21.31
ANISOU	405	СВ	ILE	52	3294	3151	1652	-449 462 -1043
ATOM	406	CG2	ILE	52	-4.238	29.178	63.931	1.000 21.29
ANISOU			ILE	52	3543	2826	1719	-362 529 -689
MOTA	407		ILE	52	-2.619	28.346	62.217	1.000 25.37
ANISOU			ILE	52	3213	3819	2608	-307 727 -1090
MOTA	408		ILE	52	-2.871	26.872	62.470	1.000 28.56
ANISOU			ILE	52	3474	3578	3798	106 178 -1110
ATOM ANISOU	409	C	ILE	52	-6.284	29.514	61.950	1.000 22.44
ANISOU	410	С 0	ILE ILE	52 52	3119 -7.072	3216	2190 62.647	-710 645 -1228 1.000 23.23
ANISOU		0	ILE	52	3390	28.856 3654	1781	-766 758 -1246
ANISOU	411	N	ASP	53	-6.519	30.754	61.530	1.000 23.33
ANISOU		N	ASP	53	2897	3064	2903	-626 700 -1361
ATOM	412	CA	ASP	53	-7.826	31.335	61.897	1.000 24.49
ANISOU		CA	ASP	53	2818	3347	3141	-759 781 -1545
ATOM	413	СВ	ASP	53	-7.942	32.781	61.411	1.000 27.43
ANISOU		CB	ASP	53	2854	3335	4235	-434 819 -1446
MOTA	414	CG	ASP	53	-9.309	33.397	61.570	1.000 30.99
ANISOU		CG	ASP	53	3166	4281	4326	36 1242 -1214
MOTA	415		ASP	53	-9.657	33.779	62.705	1.000 37.26
ANISOU			ASP	53	4369	4569	5220	153 1263 - 2733
ATOM	416		ASP	53		33.491	60.553	1.000 38.45
ANISOU			ASP	53	3393	6043	5173	810 557 -1648
ATOM ANISOU	417	C C	ASP ASP	53 53	-8.953 3028	30.495 3701	61.316 2634	1.000 24.64 -919 372 -1031
ATOM	418	0	ASP	53		. 30.327	61.915	1.000 28.52
ANISOU		ŏ	ASP	53		3835	3603	
ATOM	419	N	PHE	54	-8.744	29.978		1.000 22.04
ANISOU		N	PHE	54	2921	2974	2479	-573 174 -704
ATOM	420	CA	PHE	54	-9.772	29.187	59.432	
ANISOU	420	CA	PHE	54	2253	2879	2463	-421 771 -978
MOTA	421	CB	PHE	54	-9.423	29.030	57.942	1.000 18.45
ANISOU		CB	PHE	54	2856	1983	2171	-65 426 -518
ATOM	422	CG	PHE	54		3 28.292	57.145	1.000 21.36
ANISOU		CG	PHE	54	3063	2735	2318	-646 599 -627
ATOM	423		PHE	54		1 28.906		
ANISOU			PHE	54	3199	2783	2826	-703 -29 -624
ATOM ANISOU	424		PHE PHE	54 54	-10.29. 3482	3 27.035		1.000 23.32 -689 212 -858
ANISOU	425		PHE	54	_10 710 _10 710	2802 9 28.291	2577 56.241	
ANISOU			PHE	54	3345	3696	3008	-1418 129 - 554
ATOM	426		PHE	54		36.375		
ANISOU			PHE	54	3750	3815	2182	-1404 607 -1005
ATOM	427	CZ	PHE	54		2 27.013		1.000 26.17
ANISOU	3 427	CZ	PHE	54	3433	3830	2679	-1829 298 -813

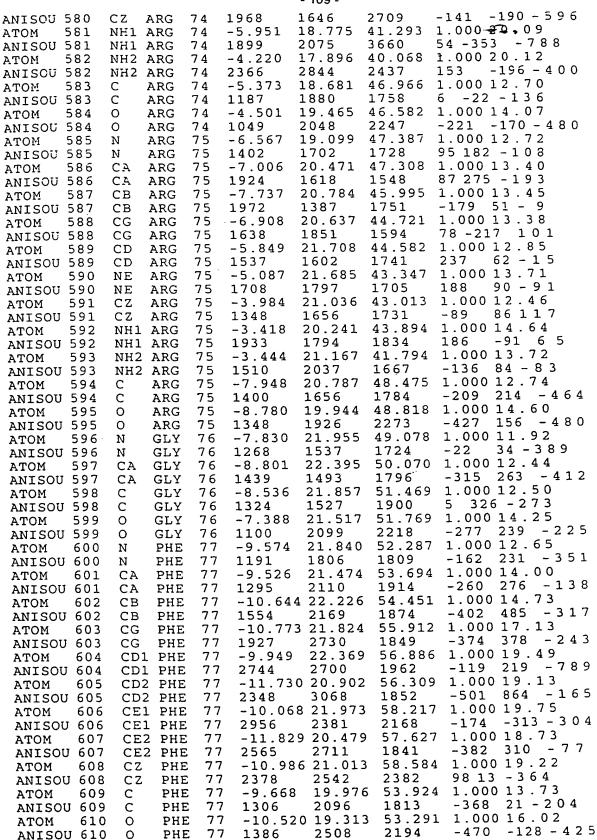
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ATOM 428			4 60.132 1.000 19.44
ANISOU 428 ATOM 429		2340 3430	1617 024 250 750
ANISOU 429			0 60.386 1.000 22.11
ATOM 430	N PHE 55		2734 -948 1018 - 1466
ANISOU 430	N PHE 55		150
ATOM 431	CA PHE 55	-8.966 25.927	1720 -666 180 -611 7 61.212 1.000 22.59
ANISOU 431 ATOM 432	CA PHE 55 CB PHE 55	3092 3671	1820 -728 381 -372
ANISOU 432	CB PHE 55 CB PHE 55	23.300	61.478 1.000 21.93
ATOM 433	CG PHE 55		1549 -692 287 -158
ANISOU 433	CG PHE 55	3034 2998	1702
ATOM 434 ANISOU 434	CD1 PHE 55 CD1 PHE 55	-7.352 24.526	5 59.057 1.000 18 72
ATOM 435	CD1 PHE 55 CD2 PHE 55		1717 -1078 586 -271
ANISOU 435	CD2 PHE 55		60.385 1.000 18.06
ATOM 436	CE1 PHE 55		1241 -926 128 -497 58.014 1.000 18.92
ANISOU 436 ATOM 437	CE1 PHE 55	2455 2761	1971 -844 436 -542
ANISOU 437	CE2 PHE 55 CE2 PHE 55	-4.672 24.124	59.352 1.000 18 58
ATOM 438	CZ PHE 55	3291 2606 -5.256 23.814	1163 -478 63 - 299
ANISOU 438	CZ PHE 55	-5.256 23.814 2660 2567	
ATOM 439	C PHE 55	-9.684 26.111	1490 -380 129 -806 62.546 1.000 24.99
ANISOU 439 ATOM 440	C PHE 55 O PHE 55	3310 4138	2046 -830 647 -415
ANISOU 440	O PHE 55 O PHE 55	$-10.532\ 25.281$ 3802 4943	62.872 1.000 30.29
ATOM 441	N GLU 56	3802 4943 -9.330 27.144	2763 -1527 1314 -1102
ANISOU 441	N GLU 56	2864 4109	2.000 25.05
ATOM 442 ANISOU 442	CA GLU 56	-9.868 27.355	2013 -634 937 -525 64.636 1.000 30.01
ATOM 443	CA GLU 56 CB GLU 56	3632 5378	2394 -1050 1465 - 9 9 4
ANISOU 443	CB GLU 56	-8.998 28.333 4531 6933	65.436 1.000 36.40
ATOM 444	CG GLU 56	-7.666 27.827	2367 -1606 1318 -1623 65.916 1.000 41.89
ANISOU 444 ATOM 445	CG GLU 56	5006 8196	2713 -1457 404 -1900
ANISOU 445	CD GLU 56 CD GLU 56	-6.787 28.880	66.575 1.000 48.94
ATOM 446	CD GLU 56 OE1 GLU 56	6081 9310 -5.694 28.515	3202 -2278 -73 - 2062
ANISOU 446	OE1 GLU 56	8034 12274	67.078 1.000 60.73 2769 -3208 -2335 2.6.6
ATOM 447 ANISOU 447	OE2 GLU 56	-7.145 30.084	2769 -3208 -2335 2 6 6 66.614 1.000 58.51
ATOM 448	OE2 GLU 56 C GLU 56	8742 9338	4151 -2088 1096 - 3951
ANISOU 448	C GLU 56 C GLU 56	-11.289 27.920 3764 4923	64.617 1.000 30.60
ATOM 449	O GLU 56	-12.058 27.542	-3// 130/ -12/1
ANISOU 449	O GLU 56	4384 5304	65.504 1.000 35.21 3690 -1136 2652 -1235
ATOM 450 ANISOU 450	N HIS 57 N HIS 57	-11.603 28.805	63.673 1.000 30.00
ATOM 451	N HIS 57 CA HIS 57	3730 4846	2823 -654 1684 - 1582
ANISOU 451	CA HIS 57	-12.854 29.559 3853 5101	63.759 1.000 33.51
ATOM 452	CB HIS 57	-12.536 31.046	3778 -519 1673 -1911 63.991 1.000 33.40
ANISOU 452 ATOM 453	CB HIS 57	3844 5183	3664 -411 1546 - 2250
ANISOU 453	CG HIS 57	-11.577 31.344	65.095 1.000 35.13
ATOM 454	CD2 HIS 57	4497 5409 -10.361 31.946	3444 -505 1340 - 1992
ANISOU 454	CD2 HIS 57	4837 5214	65.071 1.000 35.26 3345 -834 637 -1456
ATOM 455 ANISOU 455	ND1 HIS 57	-11.819 31.021	3345 -834 637 -1456 66.411 1.000 40.52
ATOM 456	ND1 HIS 57 CE1 HIS 57	6021 5885	3490 -1360 1474 - 2002
ANISOU 456	CE1 HIS 57 CE1 HIS 57	-10.798 31.410 6680 6066	67.151 1.000 42.28
ATOM 457	NE2 HIS 57	6680 6066 -9.902 31.970	3320 -1632 1099 -1772 66.362 1.000 41.69
ANISOU 457 ATOM 458	NE2 HIS 57	6377 6133	66.362 1.000 41.69 3329 -1817 407 -1148
ATOM 458	C HIS 57	-13.769 29.466	62.547 1.000 32.58
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ANISOU	458	С	HIS	57	3083	5097	4199	-729 1723 - 2066
ATOM	459	Ö	HIS	57	-14.902		62.578	1.000-33,80
ANISOU			HIS					
-		0	_	57	3121	5097	4625	-731 1865 - 2565
ATOM	460	N	GLY	58	-13.370		61.432	1.000 28.78
ANISOU		N	GLY	58	2841	4353	3742	-253 1341 -1506
ATOM	461	CA	${ t GLY}$	58	-14.326	28.685	60.332	1.000 26.99
ANISOU	461	C.A.	GLY	58	2471	3916	3869	24 1298 -1173
ATOM	462	С	GLY	58	-15.447		60.738	1.000 29.94
ANISOU		č	GLY	58	2665	4357	4353	-261 1323 - 1058
ATOM	463	Ö	GLY		-15.241			
				58			61.534	1.000 29.23
ANISOU		0	GLY	58	2976	4044	4087	-571 1192 -1297
MOTA	464	N	SER	59	-16.635		60.193	1.000 27.61
ANISOU	464	N	SER	5 9	2556	3905	4029	-108 1461 -1767
ATOM	465	CA	SER	59	-17.812	27.153	60.497	1.000 28.42
ANISOU	465	CA	SER	59	2675	4074	4049	-189 1294 -1325
ATOM	466	CB	SER	59	-19.121		60.162	1.000 28.29
ANISOU		CB	SER	59	2556	4574	3618	
ATOM	467	OG	SER	59	-19.229		58.739	1.000 28.66
ANISOU		OG	SER	5 9	3598	3742	3547	166 1729 - 867
MOTA	468	С	SER	59	-17.795	25.843	59.724	1.000 29.57
ANISOU	468	С	SER	59	3467	3990	3779	-646 1463 -1206
MOTA	469	0	SER	59	-16.990		58.810	1.000 22.72
ANISOU		0	SER	59	3054	3042	2537	-144 648 - 369
ATOM	470	N	GLU	60	-18.698		60.103	1.000 26.90
ANISOU						3900		
		N	GLU	60	2413		3907	-69 1079 - 853
ATOM	471	CA	GLU	60	-18.699		59.359	1.000 26.98
ANISOU		CA	GLU	60	2699	3515	4037	<b>-</b> 98 <b>7</b> 09 - 5 3 7
$\mathtt{MOTA}$	472	CB	GLU	60	-19.646	22.681	60.001	1.000 39.11
ANISOU	472	CB	GLU	60	5393	4393	5075	-1361 908 364
MOTA	473	CG	GLU	60	-19.011		60.917	1.000 44.63
ANISOU		CG	GLU	60	5606	5473	5878	-977 1079 1219
ATOM	474	CD	GLU	60	-17.507		60.797	1.000 48.52
ANISOU		CD	GLU	60	5714	6217	6503	-390 1207 8 7 7
ATOM	475		GLU	60	-17.030		59.684	1.000 48.11
ANISOU			GLU	60	5349	7545	5384	709 366 1951
$\mathtt{ATOM}$	476		GLU	60	-16.828	21.763	61.829	1.000 46.50
ANISOU	476	OE2	GLU	60	4926	5742	7000	1158 1550 - 1504
ATOM	477	С	GLU	60	-19.091		57.915	1.000 25.30
ANISOU	477	Ċ	GLU	60	2829	2728	4055	86 725 - 656
ATOM	478	Õ	GLU	60	-18.529		57.027	1.000 24.18
ANISOU								
		0	GLU	60	2119	2980	4091	-202 741 -752
MOTA	479	N	ALA	61	-20.032		57.716	1.000 25.58
ANISOU		N	ALA	61	2083	3206	4432	-34 612 -774
ATOM	480	CA	ALA	61	-20.495	25.212	56.368	1.000 24.05
ANISOU	480	CA	ALA	61	1838	2999	4301	228 720 -1055
MOTA	481	СВ	ALA	61	-21.670		56.459	1.000 27.53
ANISOU		CB	ALA	61	2807	1857	5797	394 704 - 606
ATOM	482	C	ALA	61	-19.385		55.500	1.000 27.31
ANISOU		C	ALA	61	3170	2572	4633	-377 1178 -1026
ATOM	483	0	ALA	61	-19.247		54.311	1.000 22.29
ANISOU	483	0	ALA	61	2363	1876	4232	42 661 - 319
ATOM	484	N	GLU	62	-18.580	26.642	56.118	1.000 22.18
ANISOU	484	N	GLU	62	2075	2258	4094	396 569 - 394
ATOM	485	CA	GLU	62		27.258	55.416	1.000 24.19
ANISOU		CA	GLU	62	2401	2603	4188	150 852 - 590
ATOM								
	486	CB	GLU			28.354	56.277	
ANISOU		CB	GLU	62	2401	2490	4485	91 1273 - 8 2 8
ATOM	487	CG	GLU	62		29.636	56.356	
ANISOU		CG	GLU	62	2542	2620	4409	353 421 -685
ATOM	488	CD	GLU	62	-17.288	30.581	57.480	1.000 29.27
ANISOU		CD	GLU	62	3284	2991	4845	621 515 -1290

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ATOM 489		U 62	-16.527 30.241 58.410 1.000 30 11
ANISOU 489 ATOM 490		J 62	3231 3067 5143 310 57
ATOM 490 ANISOU 490			-17.796 31.739 57 436 3 000 35 30
ATOM 491	02.		4832 2994 5584 863 133
ANISOU 491			$-16.409\ 26.226\ 55.025\ 1\ 000\ 21\ 70$
ATOM 492	- 020		2394 2421 3430 30.784 570
ANISOU 492		_	$-15.818\ 26.218\ 53.940\ 1.000\ 19\ 44$
ATOM 493	- 050		2095 2140 3153 301 467
ANISOU 493			$^{-16.184}$ 25.308 55.972 1 000 20 00
ATOM 494			2472 2266 2893 -74 761 -902
ANISOU 494			13.246 24.22/ 55.678 1.000 19 73
ATOM 495	CB LYS		2322 2559 2614 133 429 -903
ANISOU 495	CB LYS		1903 23.49/ 56.988 1.000 18.48
ATOM 496	CG LYS		12 046 51 24 0 -218 58 / -836
ANISOU 496			2116 2220
ATOM 497		63	12 020 02 20 20 20 20 325 -674
ANISOU 497	CD LYS		2070 4004
ATOM 498 ANISOU 498	CE LYS		-12.753 24.383 60.068 1.000 27.75
ATOM 499	CE LYS		3074 5008 2461 1220 500
ANISOU 499	NZ LYS		$-12.929\ 24.378\ 61.530\ 1.000\ 34.95$
ATOM 500	NZ LYS C LYS		31// $7579$ $2524$ $-2504.040$
ANISOU 500	C LYS		13.769 23.304 54.586 1.000 17 52
ATOM 501	O LYS		2014 2191 2453 51 529 - 691
ANISOU 501	O LYS		23.65 173.025 22.953 53.654 1.000 17.58
ATOM 502	N ARG		17 060 27 2704 138 707 -653
ANISOU 502	N ARG		2001 2452
ATOM 503	CA ARG		17 (10 -10 2)20 -14 614 -592
ANISOU 503 ATOM 504	CA ARG	64	1509 2526 3185 3.630
ATOM 504 ANISOU 504	C ARG	64	-17.471 22.634 52.194 1.000 20.42
ATOM 505	C ARG	64	2105 2436 3157 _300 33 536
ANISOU 505	O ARG	64	$-17.204\ 21.934\ 51.195\ 1.000\ 18\ 83$
ATOM 506	O ARG	64	1854 2184 3115 _434 575 3.03
ANISOU 506	CB ARG	64 64	1470 53.871 1.000 24.70
ATOM 507	CG ARG	64	10 030 3652 4263 -51 841 -909
ANISOU 507	CG ARG	64	2961 5204 5500
ATOM 508	CD ARG	64	21 21 22 2020 138 2882
ANISOU 508	CD ARG	64	
ATOM 509	NE ARG	64	21 776 2 7003 -2438 327 -1187
ANISOU 509	NE ARG	64	3917 8636 8652 -3060 3333 1073
ATOM 510 ANISOU 510	CZ ARG	64	22.014 21.84U 54.811 1 AAA 50 0 0
ATOM 511	CZ ARG	64	4438 8939 8972 -3479 1999 2400
ANISOU 511	NH1 ARG NH1 ARG	64	$-23.884\ 22.106\ 54.071\ 1.000\ 76\ 83$
ATOM 512	NH2 ARG	64 64	$\frac{9524}{13641} - \frac{952}{1872}$
ANISOU 512	NH2 ARG	64	7702 22.213 56.093 1.000 69.53
ATOM 513	N ALA	65	$\frac{9201}{17}$ $\frac{9424}{17}$
ANISOU 513	N ALA	65	1600 25.94/ 52.066 1.000 20.43
ATOM 514	CA ALA	65	17 505 04 55 3313 24 612 - 525
ANISOU 514	CA ALA	65	1640
ATOM 515	CB ALA	65	17 010 25 3020 409 184 -553
ANISOU 515 ATOM 516	CB ALA	65	1420 2019 5579 126 373 743
ATOM 516 ANISOU 516	C ALA	65	-16.118 24.549 50.168 1 000 17 89
ATOM 517	C ALA	65	1524 2099 3173 -47 108 103
ANISOU 517	O ALA	65	-15.983 24.732 48.954 1.000 18 77
ATOM 518	O ALA N VAL	65 66	1830 2178 3123 122 -8 - 229
ANISOU 518	N VAL	66 66	-15.100 24.248 50.973 1.000 17.99
ATOM 519	CA VAL	66	12 746 24 36 -196
		- 0	-13.746 24.066 50.430 1.000 16.74
	. *		



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ATOM ANISO ANISO ATOM ANISO A	0 U U U U U U U U U U U U U U U U U U U	COONN CCCCCCCCOONN CCCCCCCCCCCCCCCCCCCC	PRO	7.7.00	1618 -11.48 -11.48 -11.48 -11.78 1607 -12.43 1920 -10.83 2429 -11.33 -11.90 3534 -9.384 2183 -8.3745 -2113 -7.47 -7.47 -7.47 -8.62 -7.47 -7.47 -8.63 -7.47 -8.63 -7.47 -8.63 -7.47 -8.63 -7.47 -8.63 -7.47 -8.63 -7.47 -8.63 -7.47 -8.63 -8.63 -7.47 -8.63 -7.47 -8.63 -8.63 -7.47 -8.63 -8.63 -8.63 -7.45 -7.47 -8.63 -7.47 -8.63 -8.63 -7.47 -8.63 -8.63 -8.63 -7.43 -7.43 -8.63 -7.4	2512 16.600 2051 17.180 305	2163 9 3 1964 9 8 2285 7 8 2076 7 8 2173 8 1 7 4 6 1 9 20 26 26 21 26 2 2 1 2 2 2 2 2 2 2 2 2 2 2	-38
ATOM ANISOU ATOM ANISOU ATOM	573 573 574 574 575	0 0 N CA	MET MET ARG ARG ARG	73 73 74 74 74	-3.945 1713 -5.630 1881 -5.091	17.110 2512 16.600 2051 17.180	3067 49.498 3832 48.175 3150 46.967	-20 -269 - 175 1.000 21.20 -541 51 -1024 1.000 18.64 84 -461 543
ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU	576 576 577 577 578 578 579	CB CB CG CD CD NE NE		74 : 74 : 74 : 74 : 74 : 74 : 74 : 74 :	937 1986 -5.655 1711 -4.911 1270 -5.683 1967 -4.902	305 16.537 1434 16.934 1288 16.543 1031 16.816	169 45.704 3137 44.440 3144 43.185 3120 41.966 3075	1.000 15.73 27 - 174 1.000 16.53 -263 142 - 160 1.000 15.01 -156 279 - 554 1.000 16.10 268 -92 - 407 1.000 18.81 -432 -252 - 296 1.000 16.64



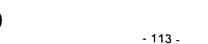
ATOM 61				- 110 -		
ATOM 61 ANISOU 61		_	-8.869	9 19.43	9 54.85	3 1 000 1 / -
ATOM 61			L543	2270	1629	
ANISOU 61	A		-9.034	18.05	3 55.27	-472·- <del>3</del> 3 - 4 9
ATOM 61			813	2310	1880	
ANISOU 61		<b>-</b>	8.001	17.08	1 54.66	508 -23 8 2 6 1.000 18.26
ATOM 61			.583	2199	3158	
ANISOU 61	4 OG1 TH	_	7.924		3 53.26	-599 334 131 6 1.000 21.81
ATOM 61		_ : -	351	1877	3057	-88 943 -370
ANISOU 61	CG2 TH	_	8.419			8 1.000 20.35
ATOM 61	5 C тн	_	855	2254	2622	-1119 1109 707
ANISOU 616	C TH		8.832 845			7 1.000 19.14
ATOM 617	7 0 ਾਸਾ		7.801	2479	1948	-1747 -471 169
ANISOU 617	7 O TH	•	781	18.311		U 1.000 22 . 04
ATOM 618	N GL	r 79 -	9.730	2889 17.203	2704	-1718 -985 7 6 3
ANISOU 618	01	792	629	2823		± 1.000 19.20
ATOM 619			9.429	16.695	1844	-1352 19 4 5
ANISOU 619	01.	79 1	800	2770	58.819 1771	
ATOM 620 ANISOU 620		79 –	8.672	15.376	58.720	-518 196 - 95
ATOM 621	- 02.	79 2	381	2874	3477	+ =
ANISOU 621	- 051	· -	9.227	14.504	58.044	-272 - 289 - 545
ATOM 622	. 011		583	2520	3514	23.57
ANISOU 622			7.494	15.236	59.319	-456 -974 - 141 1.000 22.91
ATOM 623	N LEU CA LEU		112	2900	3392	30 -206 -606
ANISOU 623	CA LEU	'	5.644	14.081	59.072	1.000 25.08
ATOM 624	C LEU		348	2777	3904	206 621 367
ANISOU 624	C LEU	,	3.372 334	13.294		1.000 24.30
ATOM 625	O LEU	80 -	.729	2762 13.812	3637	-300 480 200
ANISOU 625	O LEU	80 22	53	3017	61.291	1.000 25.14
ATOM 626 ANISOU 626	CB LEU	80 -5	.318	14.480	4283 58.415	27 145 - 5
	CB LEU	80 30	57	3326	3937	1.000 27.16
ATOM 627 ANISOU 627	CG LEU	80 -4	.411	13.338	57.933	379 918 641
ATOM 628	CG LEU CD1 LEU	80 34	74	3505	4204	1.000 29.43 287 1260 1 7 3
ANISOU 628	CD1 LEU	80 -5	.145	12.438	56.956	1.000 38.31
ATOM 629	CD2 LEU		73	3891	4993	-1554 1987 - 287
ANISOU 629	CD2 LEU	80 35	.137	13.884	57.306	1.000 29.85
ATOM 630	N GLU		.853	3919	3920	125 1307 - 264
ANISOU 630	N GLU	81 24	.033 60	12.055 2759	60.396	1.000 25.58
ATOM 631	CA GLU	81 -6	.739	11.038	4490	-196 -82 510
ANISOU 631	CA GLU	81 27	39	2692		1.000 25.98
ATOM 632	C GLU	81 -5	.299	10.536	4441 61.562	-258 -55 424
ANISOU 632 ATOM 633	C GLU	8T 58	70	3268	3848	1.000 26.28 187 407 841
ANISOU 633	O GLU		.489	10.655	60.655	187 407 841 1.000 28.19
ATOM 634	O GLU	81 37		3520	3483	
ANISOU 634	CB GLU		685	9.861	61.123	253 799 - 544 1.000 29.83
ATOM 635	CG GLU	81 35	_	2894	4906	-770 270 181
ANISOU 635	CG GLU	81 -7 81 171	241	8.832	60.098	1.000 25.34
ATOM 636	CD GLU			2915	4976	284 -1220 158
ANISOU 636	CD GLU	81 184		9.156 3405	58.649	1.000 27.00
ATOM 637	OE1 GLU		_	10.240	5012	475 -1887 - 456
ANISOU 637 ATOM 638	OE1 GLU	81 344		3091	58.324 4413	1.000 28.81
ATOM 638 ANISOU 638	OE2 GLU	81 -7.		8.273	57.814	322 -155 7 9 1
ATOM 639	OE2 GLU	81 351	4	3384	4999	1.000 31.31 162 352 100
ANISOU 639	N SER N SER		988	9.974	62.720	162 352 1 0 0 1.000 31.00
ATOM 640	N SER CA SER	82 356	_	3780	4430	-65 -30 1484
ANISOU 640	CA SER			9.422	62.959	1.000 30.29
ATOM 641	C SER			3278	4540	-157 -515 1011
		J.	721	8.150	62.150	1.000 31.76
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- 111 --102 -1104 8 4 7 4831 3241 ANISOU 641 С SER 82 3995 61.397 1.000 34,01 -4.313 7.728 642 0 SER 82 MOTA 458 -1188 134 3794 5935 3193 ANISOU 642 О SER 82 64.452 1.000 34.74 CB-3.463 9.167 SER 82 643 MOTA -232 -979 9 7 1 CB 82 4687 3907 4606 ANISOU 643 SER 64.681 1.000 41.53 644 OG SER 82 -2.360 8.305 ATOM -1958 970 236 ANISOU 644 5366 5490 4922 OG SER 82 -17.230 9.498 70.136 1.000 42.64 GLY 91 645 MOTA 7599 4086 -2166 2340 - 427 ANISOU 645 91 4516 GLY -17.485 10.892 69.789 1.000 44.91 646 CAGLY 91 MOTA 2697 -4311 -1561 565 6666 7702 GLY 91 CAANISOU 646 -16.227 11.662 69.452 1.000 38.67 GLY 91 647 С MOTA ANISOU 647 С GLY 91 5455 7587 1652 -2821 -274 -159 -15.164 11.480 70.040 1.000 32.45 648 0 GLY 91 MOTA -183 1152 - 439 ANISOU 648 91 4241 4474 3616 0 GLY -16.332 12.558 68.474 1.000 31.97 GLY 92 649 N MOTA -1382 735 -571 5904 2363 ANISOU 649 GLY 92 3881 N -15.232 13.412 68.075 1.000 33.02 92 650 CA GLY MOTA 4121 6150 -1716 851 - 956 2274 GLY92 ANISOU 650 CA. -15.223 13.696 66.572 1.000 26.22 92 С GLY 651 MOTA -885 741 -947 5046 2314 С GLY 92 2603 ANISOU 651 -16.289 13.666 65.939 1.000 23.91 GLY 92 MOTA 652 0 -680 548 -567 2490 3396 3198 ANISOU 652 GLY 92 0 -14.010 13.956 66.088 1.000 23.77 653 93 SER MOTA N -372 736 -560 2708 2405 3917 ANISOU 653 N SER 93 -13.801 14.287 64.690 1.000 23.41 93 654 CASER MOTA 2901 -386 970 -399 93 2700 3292 ANISOU 654 CA SER -12.410 13.852 64.240 1.000 24.26 655 С SER 93 MOTA -286 833 -224 2763 93 2547 3908 ANISOU 655 С SER -11.497 13.831 65.089 1.000 27.06 93 0 SER ATOM 656 3401 92 - 386 3536 3346 630 ANISOU 656 SER 93 0 -13.966 15.795 64.467 1.000 25.71 657 СB SER 93 ATOM 3735 -576 271 -506 93 2811 3225 ANISOU 657 CB SER -13.558 16.158 63.150 1.000 28.14 SER 93 658 OG MOTA -373 290 517 4284 ANISOU 658 OG SER 93 2694 3713 -12.254 13.533 62.949 1.000 24.24 659 N TYR 94 MOTA -204 791 -817 2786 3320 3104 94 ANISOU 659 N TYR -10.878 13.262 62.498 1.000 23.94 TYR 94 660 MOTA CA 95 1112 - 683  $\mathtt{TYR}$ 94 3089 2502 3505 ANISOU 660 CA -10.017 14.531 62.584 1.000 25.19 С TYR 94 661 ATOM 737 -625 94 2601 2657 4312 147 С TYR ANISOU 661 14.421 62.694 1.000 30.11 94 -8.786 TYR 0 MOTA 662 760 3 6 94 2617 5726 307 0 TYR 3095 ANISOU 662 94 -10.800 12.659 61.098 1.000 25.64 663 CB TYR MOTA -293 1331 - 525 2910 3267 ANISOU 663 CB TYR 94 3566 94 -11.600 11.410 60.876 1.000 23.22 TYR MOTA 664 CG 2768 2697 784 - 274 -69 94 3359 ANISOU 664 CG TYR -12.451 11.455 59.777 1.000 26.01 CD1 TYR 94 665 ATOM 353 - 543 2741 499 94 4410 2730 ANISOU 665 CD1 TYR -11.564 10.252 61.635 1.000 24.42 94 CD2 TYR MOTA 666 3117 3297 73 458 - 1 4 CD2 TYR 94 2866 ANISOU 666 -13.243 10.407 59.443 1.000 28.75 667 CE1 TYR 94 MOTA 434 140 -1370 4559 3328 3037 ANISOU 667 CE1 TYR 94 61.305 1.000 26.47 CE2 TYR 94 -12.375 9.159 668 MOTA -220 1227 - 718 2585 ANISOU 668 CE2 TYR 94 4707 2764 60.212 1.000 29.70 -13.209 9.247 94 669 CZTYR MOTA -1172 1103 -1447 3518 2125 ANISOU 669 CZTYR 94 5641 -14.059 8.281 59.730 1.000 34.02 670 TYR 94 MOTA OH -423 1593 - 2638 5886 94 3079 3962 OH TYR ANISOU 670 -10.628 15.714 62.561 1.000 22.61 95 671 N SER MOTA -54 59 - 338 2497 3632 ANISOU 671 N SER 95 2460

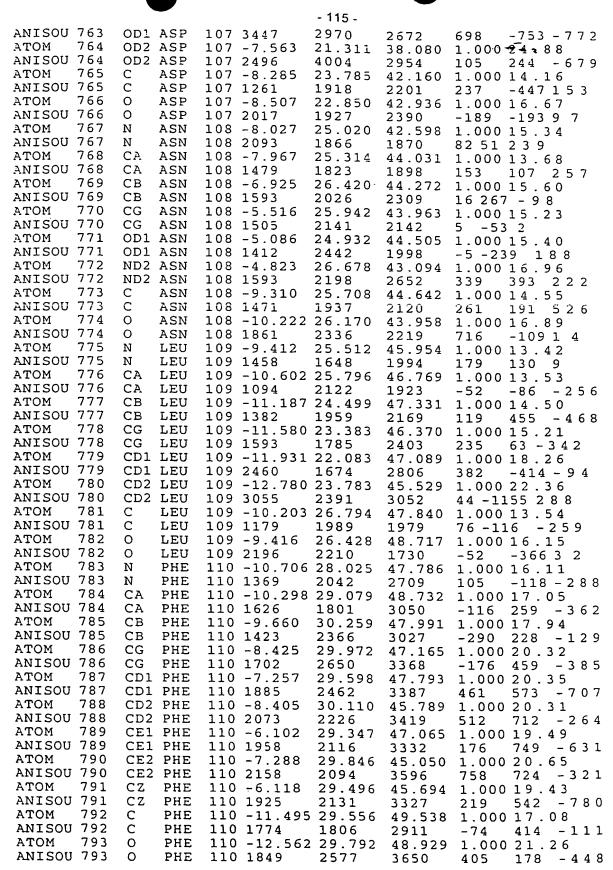
7 mov	_			- 112 -		
ATOM 672		SER 95	-9.924		5 63 354	
ANISOU 672		SER 95		2603		
ATOM 673	3 C 9	SER 95		77.106	3706	-120301 4 6
ANISOU 673	3 C 9	SER 95				
ATOM 674	109	SER 95		3478	3671	-521 -88 -85
ANISOU 674		SER 95				1.000 26,53
ATOM 675		SER 95		3242	4247	-469 - 167 - 641
ANISOU 675	<b>-</b>	ER 95		8 18.177	7 62.478	1.000 27.58
ATOM 676			3657	2556	4261	365 -379 2 8
ANISOU 676			-11.50	6 18.093	61.242	1.000 39.40
ATOM 677		ER 95	6336	4214	4421	
ANISOU 677	•	SP 96	-9.712		65.060	900 -1445 1442 1.000 25.04
ATOM 678		SP 96	2579	3688	3248	
ANISOU 678		SP 96	-9.228	16.317	66.422	-399 277 -232 1.000 24 .42
ATOM 679		SP 96	2603	3347	3330	
ANISOU 679		SP 96	-7.735	16.050	66.501	
		SP 96	2597	3228	3466	
ATOM 680		SP 96	-7.073	16.589	67.404	-471 162 -383
ANISOU 680		SP 96	2656	4047	3370.	
ATOM 681		SP 96	-9.952	15.334	33/0.	-170 160 -798
ANISOU 681	CB A	SP 96	2310	380.6		
ATOM 682	CG A	SP 96		1 15.605	3371	-423 -228 7 7
ANISOU 682	CG A	SP 96	2272	4334		1.000 26.77
ATOM 683	OD1 A	SP 96		5 16.723	3566	-362 -240 7 1 6
ANISOU 683	OD1 A	SP 96	3267	10./23		1.000 33.94
ATOM 684	OD2 A	SP 96		4894	4733	647 204 569
ANISOU 684	OD2 A	SP 96	3624	3 14.646		1.000 32.65
ATOM 685		(R 97	2024	4709	4072	-1032 1446 - 202
ANISOU 685		(R 97	-7.254	15.226	65.581	1.000 22.21
ATOM 686			2292	3389	2760	-376 -77 -102
ANISOU 686			-5.835	14.852	65.583	1.000 23.71
ATOM 687	C TY		2480	3542	2987	-27 106 644
ANISOU 687			-5.026	15.828	64.743	1.000 23.06
ATOM 688			2363	3754	2647	-410 -78 350
ANISOU 688			-3.992	16.327	65.230	1.000 24.29
ATOM 689			2205	3845	3178	-133 -230 7 4
ANISOU 689	CB TY		-5.585	13.451	65.035	1.000 28.38
	CB TY		3230	3324	4229	
ATOM 690 ANISOU 690	CG TY		-4.132	13.025	65.082	
	CG TY		3278	4101	4161	1.000 30 . 37 766 -191 6 7 1
	CD1 TY	R 97	-3.511	12.691	66.285	
ANISOU 691	CD1 TY	R 97	2878	4475	4119	1.000 30.19
ATOM 692	CD2 TY	R 97	-3.370	12.945	63.922	1106 151 951
ANISOU 692	CD2 TY	R 97	3317	4005	03.922	1.000 29.79
ATOM 693	CE1 TY	R 97	-2.178	12 204	3997	53 - 253 544
ANISOU 693	CE1 TY	R 97	2554	4771		1.000 32.77
ATOM 694	CE2 TY	R 97	-2.043	12.553	5126	574 -68 763
ANISOU 694	CE2 TY		3536		63.955	1.000 32.68
ATOM 695	CZ TY		-1.445	3793	5087	403 353 323
ANISOU 695	CZ TY		2633	12.228	65.157	1.000 33.00
ATOM 696	OH TY			4284	5622	1066 264 456
ANISOU 696	OH TY		-0.121	11.845	65.156	1.000 42.66
ATOM 697	CB SE		2572	5373	8264	1161 764 1277
ANISOU 697	~ ~	_	-3.465	16.575	62.134	1.000 23.20
ATOM 698			2461	2766		105 2 - 544
ANISOU 698	OG SE		-3.632	15.649		1.000 26.49
ATOM 699	OG SE	_	3824	3059		-154 238 -457
ANISOU 699	C SE		-5.694	17.744		1.000 18.66
	C SE	R 98	2301	2150		
	O SE	R 98	-6.768	17.212		
ANISOU 700	0 SE:	R 98	3042	2245		1.000 20.88
ATOM 701	N SE	R 98	-5.457	16.110		-945 -249 1 8 1
ANISOU 701	N SE	R 98	2816	3227		1.000 23.62
ATOM 702	CA SE			17.143	_	-441 -395 6 0 5
					62.741	1.000 21.31
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ANISOU 702	CA SER	98 2430	2687 2982	133 153 294
ATOM 703	N MET	99 -5.307	18.891 61.148	1.000 1-8 -68
ANISOU 703	N MET	99 2392	2722 1984	-978 -366101
ATOM 704	CA MET	99 -6.047	19.560 60.075	1.000 17.84
ANISOU 704		99 2431	2620 1726	-945 -212 - 17
ATOM 705	CB MET	99 -6.819	20.779 60.585	1.000 19.71
ANISOU 705	CB MET	99 2348	2968 2173	-679 25 6 4
ATOM 706	CG MET	99 -8.052	20.392 61.374	
ANISOU 706	CG MET	99 2360	3055 3582	-504 393 489
ATOM 707		99 -9.031	21.821 61.911	1.000 22.33
ANISOU 707	SD MET	99 2569	3383 2534	-522 170 -120
ATOM 708	CE MET	99 -8.148	22.225 63.419	
ANISOU 708	CE MET	99 6485	4165 3401	-225 - 1904 - 23
ATOM 709		99 -5.070		
ANISOU 709	C MET	99 2269	2488 1776	-960 -194 - 201
ATOM 710	O MET	99 -3.964		1.000 16.93
ANISOU 710	O MET	99 1932	2583 1919	-367 -208 - 24 <u>1</u>
ATOM 711		100 -5.486		1.000 20.00
ANISOU 711		100 3178	2683 1739	-1753 -358 1 6 6
ATOM 712		100 -4.645		1.000 16.64
ANISOU 712		100 2213	2294 1817	-924 -563 4 6 8
ATOM 713		100 -4.291		1.000 17.74
ANISOU 713		100 2161	2174 2407	560 -765 1 0 5 3
ATOM 714		100 -3.035		1.000 33.56
ANISOU 714		100 5244	3511 3997	414 1509 6 0 1
ATOM 715		100 -5.347		
ANISOU 715		100 1879	1415 1829	-68 240 -91
ATOM 716		100 -6.585		
ANISOU 716		100 1880	1952 1673	
ATOM 717		101 - 4.589		
ANISOU 717		101 1721	1677 1673	
ATOM 718		101 -5.016		1.000 10.27
ANISOU 718		101 926 14		
ATOM 719		101 -5.102		1.000 13.60
ANISOU 719		101 1626	1513 2027	
ATOM 720		101 -5.498		
ANISOU 720		101 2373	1509 2694	
ATOM 721		101 -6.815		
ANISOU 721		101 2464		90 -227 5 5
ATOM 722		101 -7.307		
ANISOU 722		101 2755		36 -416 122
ATOM 723 ANISOU 723		101 -4.616 101 3032	_ ,	
ATOM 724			1533 2847	-1143 -594 4 7 5
ANISOU 724		101 -5.065		
ATOM 725		101 2802 101 -6.414	1949 3211	238 112 769
ANISOU 725				
ATOM 726		101 3238	2291 3126	-1228 -919 6 2 4
ANISOU 726	OH TYR OH TYR	101 -6.875		
ATOM 727	C TYR	101 3141 101 -4.041		-14 -129 4 2 9
ANISOU 727	C TYR	101 1223		
ATOM 728	O TYR		1398 1654	-323 103 -252
ANISOU 728	O TYR	101 -2.823 101 1114		
ATOM 729	N SER	102 -4.542		-87 130 - 20
ANISOU 729	N SER	102 -4.542		
ATOM 730	CA SER	102 1355		
ANISOU 730	CA SER	102 -3.752	2 21.802 50.235 1263 1568	
ATOM 731	CB SER	102 1144		62 -1 -125
ANISOU 731	CB SER	102 1668	7 20.343 49.908 1212 2234	3 1.000 13.46 324 105 -301
ATOM 732	OG SER	102 1000		
ANISOU 732	OG SER	102 2291	1313 2637	-122 -43 9 6
144100 /32	UG JER	TO 6 6631	1313 2037	-122 -43 3 0

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ATOM ANISOU	7.734 $7.734$ $7.7334$ $7.7336$ $7.7338$ $7.7$	OG1 CG2	RRRRTTTTTTTTTTTTTTTTYYYYYYRRRRRRRRRRRRR	102 102 103 103 103 103 103 103 103 103 103 103	-3.004 1554 -3.188 1663 -3.215 2439 -1.929 2509 -2.136 2235 -2.365 2319 -2.152 1420 -1.120 1094 -2.418 1493 -1.533 1075 -1.624 1909 -2.033 1628 -1.242 1829 -1.218 1977 -0.359 1936 -0.884 1738 1.092 1918 -2.603 1989 -2.730	22.668 1500 23.148 1410 22.871 1722 23.603 1681 25.12 163.4 25.34 25.61 24.65 28.70 21837 22.573 1891 23.650 23.459 2188 24.62 25.45 2188 24.62 25.45 2188 2188 22.73 2182 22.87 25.45 22.87 25.45 22.87 25.45 22.87 260 24.88 22.871 25.82 269 24.88 22871	1614 48.784 198.888 140.93 146.97 146.57 147.565 147.59 145.17 146.17 146.17 147.65 147.65 147.65 147.65 147.61	90 -66 2 4 9 1.000 12.33 -262 -10 -2 4 6 1.000 12.92 22 47 - 7 C 1.000 17.51 -363 812 - 4 4 1.000 20.07 -538 688 3 7 6 1.000 18.10 -3 -334 - 352 1.000 18.09 -187 -718 - 2 1 4 1.000 12.57 -19 -53 2 3 8 1.000 12.57 -155 -165 2 7 6 1.000 12.83 237 -124 - 3 4 1.000 12.65 -93 -37 2 4 2 1.000 14.36 -265 -294 1 4 2 1.000 15.69 163 -197 2 1 3 1.000 15.69 163 -197 2 1 3 1.000 15.69 163 -197 2 1 3 1.000 15.69 163 -197 2 1 3 1.000 15.69 163 -197 2 1 3 1.000 15.69 163 -197 2 1 3 1.000 15.61 -37 -106 5 5 4 1.000 15.61 -37 -285 1 5 1 1.000 17.47 -293 -227 5 2 7 1.000 14.73 122 -340 1 9 9 1.000 19.91
						2188	1544	-93 <b>-</b> 37 242
ATOM	745						1544	-93 <b>-</b> 37 242
				104	1909	1985		
ANISOU				104	-2.033	25.700		1.000 15.69
		N	THR	105	-1.242	24.397		
				105	1829	2182	1504	-59 -375 3 1 9
	748	CA		105	1977			
				105	-0.359	25.083	39.039	1.000 15.61
MOTA	750			105	-0.884			-37 -106 5 5 4
ANISOU				105	1738	2260		
ANISOU							39.369	1.000 17.47
		С	THR	105	-2.603	25.828		
ATOM							1913	122 -340 1 9 9
ANISOU	753	0	THR	105	2579		39.174 2632	1.000 19.91 23 -437 1004
ATOM ANISOU	754 754	N	ALA ALA	106. 106	-3.587	24.960	39.913	1.000 16.57
ATOM	755	CA	ALA	106	-4.975	2413 25.167	2047 39.465	2 -260 661 1.00014.94
ANISOU ATOM	755 756	CA CB	ALA ALA	106	1975	1904	1798	105 -456 3 6 5
ANISOU	756	CB	ALA	106	-5.054 2006	24.945 2862	37.965 1876	1.000 17.75
ATOM ANISOU	757 757	C C	ALA	106	-5.942	24.251	40.222	140 -201 - 3 2 1.000 16.26
MOTA	758		ALA ALA	106	1710 -5.498	2174 23.398	2293	327 -127 4 9 1
ANISOU ATOM		0	ALA	106	1622	1971	41.013 1945	1.000 14.57 213 -21 337
ANISOU			ASP ASP	107 107	-7.253	24.410	40.008	1.000 16.71
ATOM	760	CA	ASP	107	-8.310	2096 23.638	2485 40.633	540 -22 3 0 4 1.000 16.10
ANISOU ATOM			ASP ASP	107	1696	2175	2246	51 -485 - 14
ANISOU	761	CB	ASP	107	-8.231 1299	22.171 2385	40.211 2808	1.000 17.09
ATOM ANISOU		CG	ASP	107	-8.418	21.966	38.720	144 -203 - 399 1.000 21.54
		CG OD1	ASP ASP	107 : 107 :	2385 -9.452	2894	2906	84 -317 -722
			_		=	22.443	38.189	1.000 23.92



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ATOM	794	N	PRO	11:	1 -11.40	6 29.717	50.851	1.000 19.41
ANISO		N	PRO	11:	l 2279	2110	2985	-386 <del>-519</del> -314
ATOM	795	CD	PRO	111	L -10.27	8 29.322	51.705	
ANISO ATOM		CD	PRO	111	L 2773	1880	2640	
	796	CA	PRO	111	-12.54	9 30.252	51.604	-417 255 -514 1.000 21.47
ANISO		CA	PRO	111	. 3026	1924	3206	
ATOM	797	CB	PRO	111	-12.16	7 30.007	53.055	-50 728 -635 1.000 23.63
ANISON ATOM		CB	PRO	111	. 3789	2054	3137	
ANISO	798	CG	PRO	111	10.77	5 29.535	53.100	334 776 - 575 1.000 22.33
ATOM	799	CG	PRO	111	. 2767	2908	2809	
ANISO		C	PRO	111	-12.82	8 31.739	51.433	-1006 623 -414 1.000 23.88
ATOM	800	C	PRO	111	3139	2049	3887	79 -142 -479
ANISO		0	PRO	111	-13.91	9 32.194	51.834	1.000 26.77
ATOM	801	N	PRO SER	111	3800	2818	3555	992 -91 -397
ANISOU		N	SER	112	-11.90	5 32.517		1.000 25.19
ATOM	802	CA	SER	112		2269	3788	-247 -856 2 8 2
ANISOL		CA	SER	112	-12.300	33.919	50.631	1.000 26.43
ATOM	803	CB	SER	112		2655	4734	496 1364 456
ANISOU		CB	SER	112	-12.50	34.712	51.912	1.000 33.37
ATOM	804	OG	SER		3122	3663	5895	172 2582 - 510
ANISOU		ŌĞ	SER	112	-11.322 6530		52.688	1.000 36.94
ATOM	805	Ċ	SER	112	-11.262	2154	5351	1399 206 -415
ANISOU	805	Ċ	SER	112	2613	34.587	49.723	1.000 26.62
ATOM	806	0	SER	112		2546 34.029	4956	1021 1668 651
ANISOU		0	SER		2241	2782	49.414	1.000 22.81
ATOM	807	N	$\mathtt{GLY}$	113	-11.570	2702	3645 49.279	800 837 -400
ANISOU		N	$\mathtt{GLY}$	113	2937	2947	5108	1.000 28.93
ATOM	808	CA	${ t GLY}$	113	-10.659	36.478	48.365	1008 1175 1198
ANISOU		CA	${ t GLY}$	113	2992	3606	5102	1.000 30 . 79 381 798 1400
ATOM ANISOU	809	C	GLY		-9.362	36.829	49.070	381 798 1400 1.000 31.83
ATOM		C	GLY	113	3297	3919	4878	262 897 528
ANISOU	810 810	0	GLY	113	-8.294	36.790	48.459	1.000 25.85
ATOM	811	O N	GLY	113	2920	2317	4585	857 450 - 203
ANISOU		N	ASP ASP	114	-9.479	37.145	50.365	1.000 29.56
ATOM	812	CA	ASP	114	3487	2877.	4868	866 1104 7 6 0
ANISOU	812	CA	ASP	114	-8.257 3189	37.463	51.122	1.000 26.15
ATOM	813	CB	ASP	114	-8.628	2680	4066	1028 1584 5 4 2
ANISOU	813	CB	ASP	114	5580	37.937	52.526	1.000 33.81
ATOM	814	CG	ASP	114	-7.904	2697	4569	1774 1691 - 240
ANISOU		CG	ASP	114	6798	39.232 3734	52.840	1.000 40.77
ATOM	815	OD1	ASP		-8.330	40.277	4960	719 693 -248
ANISOU		OD1	ASP	114	6014	2534	52.295	1.000 48.61
ATOM	816	OD2	ASP	114	-6.932	39.178	9920 53.622	1703 931 - 913
ANISOU		OD2		114	5258	7609	7783	1.000 54.35 -868 495 1602
MOTA	817	C	ASP	114	-7.310	36.281	51.231	-868 495 1602 1.000 23.05
ANISOU ATOM		C	ASP	114	2621	2102	4033	444 1874 3 4 0
ANISOU	818	0	ASP	114	-6.111	36.371	50.955	1.000 22.05
ATOM	819	0	ASP	114	2423	2277	3677	131 1411 - 461
ANISOU	810	N N	PHE	115	-7.854	35.160	51.637	1.000 23.21
ATOM	820		PHE	115	2945	1890	3984	-130 1293 - 228
ANISOU	820	CA CA	PHE PHE	112	-7.120	33.896	51.690	1.000 19.93
ATOM	821	CB	PHE	115	2562	1908	3102	-198 655 -294
ANISOU	821	CB	PHE	115	-8.085 2378	32.792	52.157	1.000.19.49
ATOM	822	CG	PHE		-7.523	1754	3275	64 881 - 314
ANISOU	822	CG	PHE		-7.523 2053	31.445	52.540	1.000 17.25
ATOM	823	CD1			-7.637	1589	2912	-56 348 -695
ANISOU	823	CD1	PHE	115	2728	30.951 1539	53.833	1.000 19.00
ATOM	824	CD2	PHE	115	-6.868	30.634	2950	73 496 - 683
				_		50.054	51.615	1.000 17.88

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ANISOU		CD2			1933	1931	2927	7 298 - 810
ATOM	825	CEl			-7.100	29.711	54.163	1.000-2-025
ANISOU	825	CE1		115	2825	1825	3042	317 341 -575
ATOM ANISOU		CE2	PHE	115	-6.338 1865	29.412 2158	51.955 3237	1.000 19.11 336 351 -885
ATOM	827	CZ	PHE		-6.452	28.936	53.233	1.000 19.39
ANISOU		CZ	PHE	115	2068	1910	3390	320 248 -669
ATOM	828	С	PHE	115	-6.506	33.624	50.327	1.000 17.86
ANISOU		C	PHE		1964	1945	2878	61 344 1 6
MOTA	829	0	PHE		-5.324	33.315	50.271	1.000 17.34
ANISOU ATOM	830	O N	PHE GLU	115	1868 -7.310	2107 33.683	2613 49.263	-132 179 157
ANISOU		N	GLU		1921	1934	3065	1.000 18.21 547 281 6 2
ATOM	831	CA	GLU		-6.848	33.387	47.907	1.000 19.99
ANISOU		CA	GLU	116	2128	2618	2851	81 231 2 2 2
MOTA	832	CB	GLU		-7.968	33.605		1.000 18.61
ANISOU		CB	GLU		2058	1952	3060	231 244 270
ATOM ANISOU	833 833	CG CG	GLU GLU		-7.398 1813	33.378 2288	45.482 2971	1.000 18.61 295 -32 - 33
ATOM	834	CD	GLU		-8.442	33.230	44.412	1.000 22.40
ANISOU		ÇD	GLU		1908	3193	3410	-122 -278 - 9 1
MOTA	835		GLU	116	-9.654	33.272	44.678	1.000 30.82
ANISOU			GLU		1793	4465	5452	273 -414 - 24
ATOM	836		GLU		-8.085	33.063	43.225	1.000 30.24
ANISOU ATOM	837	C	GLU GLU		3333 -5.620	5132 34.211	3026 47.535	382 -658 3 2 7 1.000 18.82
ANISOU		C	GLU		2090	2069	2990	294 119 487
ATOM	838	Ō	GLU		-4.605	33.701	47.049	1.000 17.41
ANISOU		0	GLU		2228	1780	2606	45 259 2 8 2
ATOM	839	N	ARG		-5.660	35.508	47.777	1.000 21.02
ANISOU ATOM	840	N CA	ARG ARG	117	2313 -4.560	2185 36.420	3487	408 220 9 0 1.000 21.35
ANISOU		CA	ARG		2337	1800	47.431 3976	466 147 - 31
ATOM	841	C	ARG		-3.291	36.054	48.192	1.000 20.52
ANISOU		С	ARG		2292	2124	3380	353 288 - 10
ATOM	842	0	ARG		-2.186	35.969	47.636	1.000 18.96
ANISOU		0	ARG		2223	1664	3316	138 318 231
ATOM ANISOU	843 843	CB CB	ARG ARG		-4.971 3237	37.885 1900	47.693 4587	1.000 25.59 929 1882 6 3 2
MOTA	844	CG	ARG		-3.881	38.908	47.478	1.000 32.57
ANISOU	844	CG	ARG		5212	1925	5237	-281 1083 6 2 3
MOTA	845	CD	ARG	117	-4.325	40.323	47.859	1.000 36.56
ANISOU		CD	ARG		6009	2157	5.724	149 1774 6 6 3
ATOM ANISOU	846 846	NE NE	ARG ARG		-5.162 7200	40.335 3742	49.056 5940	1.000 44.43 -96 2344 - 15
ATOM	847	CZ	ARG		-4.763	40.501	50.306	1.000 45.48
ANISOU		CZ	ARG		6422	4804	6054	-370 2388 - 283
ATOM	848		ARG		-3.484	40.683	50.619	1.000 53.21
ANISOU			ARG		6867	6451	6900	-2543 2487 3 5 4
ATOM ANISOU	849		ARG ARG		-5.647 6265	40.487	51.301	1.000 50.00
ATOM	850	Nn2	ILE		-3.439	6511 35.832	6220 49.493	224 2433 - 1534 1.000 19.30
ANISOU		N	ILE		2275	1838	3221	128 407 - 645
ATOM	851	CA	ILE	118	-2.275	35.527	50.331	1.000 18.25
ANISOU		CA	ILE		2376	1745	2811	78 530 - 449
	852	CB	ILE		-2.665	35.597	51.820	
ANISOU ATOM	852 853	CB	ILE		2201 -1.712	1726 34.851	3003 52.732	346 906 - 306 1.000 18.49
ANISOU			ILE		2077	2158	2792	-202 308 -530
ATOM	854		ILE		-2.877	37.031	52.368	
ANISOU	854	CG1	ILE		4436	1808	3136	284 1382 - 414
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MOTA	855		ILE	118	3 -3.786	37.025	53.582	1 000 20 62
ANISOU			ILE	118	6169	3096	1994	1.000 29 .63 189 - <del>1</del> 258 - 1068
ATOM	856	C	ILE	118	-1.692	34.172	49.959	1.000 15.65
ANISOU ATOM		C	ILE		2316	1549	2082	=89 573 -117
ANISOU	857	0	ILE	118	-0.463	34.035	49.802	1.000 14.59
ATOM	858	0	ILE	118	2240	1255	2051	16 286 2 1 4
ANISOU		N N	TRP TRP	119	-2.523	33.139	49.784	1.000 14.44
ATOM	859	CA	TRP	119	2125	1592	1771	47 128 - 7 1
ANISOU		CA	TRP	110	-2.010 1712	31.795	49.518	1.000 13.68
ATOM	860	СB	TRP		-3.089	1529 30.755	1957	-61 220 4 0
ANISOU		CB	TRP	119	1819	1729	49.932 2123	1.000 14.93
ATOM	861	CG	TRP	119	-2.864	30.482	51.420	-234 295 - 35 1 000 16 10
ANISOU		CG	TRP	119	1640	2364	2146	1.000 16.19 -168 582 167
ATOM	862		TRP	119	-2.116	29.430	51.993	-168 582 167 1.000 20.41
ANISOU ATOM	863		TRP		3189	2414	2151	202 523 4 0 5
ANISOU		CEZ	TRP TRP	119	-2.177	29.580	53.392	1.000 19.84
ATOM	864	CE3	TRP	119	3536 -1.390	1818	2184	-439 234 137
ANISOU		CE3	TRP	119	5382	28.357	51.456	1.000 23.94
ATOM	865		TRP		-3.340	1647 31.223	2068	561 126 400
ANISOU	865		TRP	119	3207	2343	52.460 2069	1.000 20.05
ATOM	866	NE1	TRP	119	-2.938	30.689	53.649	-9 189 <i>-</i> 139
ANISOU		NE1	TRP	119	2806	2726	2188	1.000 20.32 -96 -68 -185
ATOM	867	CZ2	TRP	119	-1.547	28.714	54.281	1.000 22.12
ANISOU ATOM	868	CZ2	TRP		4071	2256	2078	-17 105 2 2
ANISOU		C23	TRP TRP	119	-0.761	27.490	52.332	1.000 21.52
ATOM	869	CH2	TRP		4214 -0.847	2168	1794	311 -193 1 9 7
ANISOU		CH2		119	5349	27.674 2047	53.715	1.000 24.34
ATOM	870	С	TRP		-1.521	31.634	1850 48.095	329 148 183
ANISOU		C	TRP	119	2180	1259	1985	1.000 14.27 -187 334 -65
ATOM	871	0	TRP	119	-0.569	30.865	47.855	-187 334 - 65 1.000 14.73
ANISOU ATOM	871 872	0	TRP	119	1996	1653	1946	-67 362 101
ANISOU		N N	THR	120	-2.109	32.325	47.116	1.000 13.99
MOTA	873	CA	THR THR		2231 -1.541	1237	1848	106 627 -137
ANISOU		CA	THR		1903	32.275	45.762	1.000 15.19
ATOM	874	CB	THR		-2.492	2093 32.983	1774	9 435 - 242
ANISOU		CB	THR	120	1934	2304	44.787 1995	1.000 16.41
ATOM	875	OG1	THR		-3.738	32.297	44.766	-331 152 6 6 1.000 18.53
ANISOU		OG1		120	1891	2288	2863	-236 195 407
ATOM ANISOU	876	CG2	THR	120	-1.974		43.358	1.000 18.02
ATOM	877	CG2			2135	2602	2108	324 322 318
ANISOU		C C	THR THR		-0.145	32.870	45.727	1.000 14.19
ATOM	878	Ō	THR		1868 0.756	2050	1475	87 285 - 167
ANISOU		ŏ	THR	120	1864	32.299 1692	45.078	1.000 13.62
MOTA	879	N	GLN	121	0.114	33.962	1620	301 354 217
ANISOU		N	GLN	121	1721	1672	46.429 2136	1.000 14.55 304 175 - 67
ATOM	880		GLN	121	1.459	34.548	46.483	304 175 - 67 1.000 15.80
ANISOU ATOM		CA	GLN	121	2067	1666	2271	-18 -119 3 6 2
ANISOU	881		GLN	121	2.465	33.642	47.176	1.000 13.73
ATOM			GLN		1747	1665	1806	-30 18 1 1 4
ANISOU			GLN GLN	121	3.603	33.452	46.685	1.000 15.36
ATOM			GLN	121	2063 1.315	1688	2084	48 360 - 4 4
ANISOU			GLN	121	2537	35.918 1426	47.154	1.000 18.85
ATOM	884		GLN	121	2.639	36.558	3200 47.543	-73 -5 3 5 6 1 000 1 8 0 8
ANISOU	_	CG	GLN	121	2507	1788	2878	1.000 18.88 59 9 - 248
ATOM	885	CD	GLN	121	3.468		46.337	1.000 20.70
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ANISOU 885 CD GLN ATOM 886 OE1 GLN ANISOU 887 NE2 GLN ATOM 888 N TYR ANISOU 888 N TYR ANISOU 889 CA TYR ANISOU 889 CA TYR ANISOU 889 CA TYR ANISOU 890 CB TYR ANISOU 891 CG TYR ANISOU 891 CG TYR ANISOU 892 CD1 TYR ANISOU 892 CD1 TYR ANISOU 893 CE1 TYR ANISOU 893 CE1 TYR ANISOU 893 CE1 TYR ANISOU 894 CD2 TYR ANISOU 895 CE2 TYR ANISOU 895 CE2 TYR ANISOU 896 CZ TYR ANISOU 897 OH TYR ANISOU 897 OH TYR ANISOU 896 CZ TYR ANISOU 897 OH TYR ANISOU 897 OH TYR ANISOU 898 C TYR ANISOU 897 OH TYR ANISOU 898 C TYR ANISOU 899 O TYR ANISOU 899 O TYR ANISOU 899 O TYR ANISOU 898 C TYR ANISOU 899 O TYR ANISOU 899 O TYR ANISOU 899 O TYR ANISOU 899 O TYR ANISOU 898 C TYR ANISOU 899 O TYR ANISOU 899 O TYR ANISOU 900 N PHE ANISOU 900 N PHE ANISOU 901 CA PHE ANISOU 901 CA PHE ANISOU 902 CB PHE ANISOU 903 CG PHE ANISOU 904 CD1 PHE ANISOU 905 CD2 PHE ANISOU 905 CD2 PHE ANISOU 906 CE1 PHE	121       2584       2138         121       2.935       37.088         121       2695       2822         121       4.779       37.101         121       2426       3344         122       2.081       33.054         122       1.747       1514         122       2.896       32.102         122       1901       1643         122       2.211       31.724         122       2.994       30.808         122       1.966       1681         122       1.788       1972         122       1.788       1972         122       1.31       2050         122       1.31       2050         122       1.34       2050         122       1.31       2050         122       1.31       2050         122       1.34       2050         122       1.31       2050         122       1.34       29.619         122       3.08       1366         122       1.413       29.101         122       2.985       1.742         122       1.833	3142
ATOM 900 N PHE ANISOU 900 N PHE	122 1896 1861 123 2.224 30.269 123 1950 1297	1656 339 -242 2 1 6 47.573 1.000 11.28 1041 6 -151 1 8 5
ANISOU 901 CA PHE ATOM 902 CB PHE ANISOU 902 CB PHE	123 1731 1219 123 1.139 28.719 123 2048 1550	1640 64 -60 2 6 46.024 1.000 13.86 1666 -104 -276 - 8 2
ANISOU 903 CG PHE ATOM 904 CD1 PHE ANISOU 904 CD1 PHE	123 2173 1677 123 1.281 26.234 123 1857 1563	1637
ANISOU 905 CD2 PHE ATOM 906 CE1 PHE ANISOU 906 CE1 PHE ATOM 907 CE2 PHE	123 1450 2164 123 1.468 25.141 123 2282 1819 123 1.715 26.559	1634 -420 -295 -248 44.795 1.000 17.16 2418 130 -855 -644 42.916 1.000 18.31
ANISOU 907 CE2 PHE ATOM 908 CZ PHE ANISOU 908 CZ PHE ATOM 909 C PHE ANISOU 909 C PHE ATOM 910 O PHE	123 1.706 25.295 123 1442 2382 123 3.489 29.511 123 2004 1472	2201 -1053 172 -845 43.445 1.000 16.71 2526 -36 -306 -1077 45.581 1.000 13.48 1645 236 157 1 8 45.242 1.000 13.07
ANISOU 910 O PHE ATOM 911 N ASP ANISOU 911 N ASP ATOM 912 CA ASP ANISOU 912 CA ASP	123 1591 1498 124 3.294 30.684 124 1490 1575 124 4.207 31.036	1876
ATOM 913 CB ASF ANISOU 913 CB ASF ATOM 914 CG ASF ANISOU 914 CG ASF ATOM 915 OD1 ASF	124 3.708 32.352 124 2650 1970 124 4.470 32.708 124 5327 2099	2389 458 398 344 43.242 1.000 18.95 2580 656 -63 926 41.989 1.000 27.54 3036 -123 939 880 41.023 1.000 37.04
ANISOU 915 OD1 ASE	124 6362 3225	4485 108 2616 - 3 3 1

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ATOM	916		ASP	124	4.985	33 843	42.011	1 000 30 60
JOSINA		OD2	ASP		4724	3509	4151	
ATOM	917	С	ASP		5.645	31.164	44.328	-1539 234 ,851
ANISOU	917	С	ASP		1493	1721		1.000 14.49
ATOM	918	0	ASP		6.591	30.721	2293 43.674	22, 403 402
ANISOU	918	0	ASP		1477	1363	2679	1.000 14.52
ATOM	919	N	ARG		5.866	31.777		289 497 3 0 7
ANISOU	919	N	ARG	125	1501	1271	45.499	1.000 14.03
ATOM	920	CA	ARG		7.214	31.863	2558	353 398 414
ANISOU	920	CA	ARG	125	1642	1625	46.044	1.000 16.40
MOTA	921	С	ARG		7.828	30.494	2963	194 178 226
ANISOU	921	С	ARG	125	1396	1688	46.346	1.000 14.69
MOTA	922	0	ARG	125	8.999	30.245	2496	232 -25 153
ANISOU	922	0	ARG	125	1279	1656	46.034 2424	1.000 14.10
ATOM	923	CB	ARG	125	7.213	32.705		7 -205 -201
ANISOU	923	CB	ARG	125	1950	1902	47.318 3035	1.000 18.13
ATOM	924	CG	ARG		7.045	34.193		787 -81 4 6
ANISOU	924	CG	ARG	125	2232	1780	47.041	1.000 23.51
ATOM	925	CD	ARG	125	8.391	34.815	4919	883 -36 -225
ANISOU	925	CD	ARG	125	3596	2824	46.694	1.000 29.33
ATOM	926	NE	ARG	125	8.194	36.262	4724	-667 237 -187
ANISOU	926	NE	ARG	125	4350	2766	46.803	1.000 32.99
ATOM	927	CZ	ARG	125	8.868	37.153	5418	-678 -1642 156
ANISOU	927	CZ	ARG	125	2292	2758	47.495	1.000 27.38
MOTA	928		ARG		9.916	36.821	5353	-276 -580 - 246
ANISOU	928		ARG	125	4611	3604	48.235	1.000 38.55
ATOM	929		ARG	125	8.491	38.423	6433	449 -2476 -669
ANISOU	929	NH2	ARG	125	4062	2570	47.442	1.000 30.26
ATOM	930	N	GLN		7.065	29.573	4865	-369 -835 3 6 3
ANISOU	930	N	GLN	126	1316	1376	46.920	1.000 12.36
ATOM	931	CA	GLN		7.524	28.201	2002	248 -63 -264
ANISOU	931	CA	GLN		1765	1323	47.153	1.000 13.39
MOTA	932	CВ		126	6.363	27.455	1999	219 -355 - 377
ANISOU	932	CB	AGLN	126	2422	1391	47.828	0.500 16.24
ATOM	933	CG	AGLN	126	6.149	27.758	2357	188 202 - 192
ANISOU	933	CG	AGLN	126	2761	2021	49.284	
ATOM	934	CD	AGLN	126	7.077	27.146	2371	68 233 - 210
ANISOU	934	CD	AGLN	126	3578	27.146	50.298	0.500 23.94
MOTA	935	OE1	AGLN	126	7.181	27.683	2774	-604 -757 3 3
ANISOU	935	OE1	AGLN	126	6788	3731	51.419	0.500 35.94
MOTA	936	NE2	AGLN	126	7.774	26.055	3136	-578 -1567 -478
ANISOU	936	NE2	AGLN	126	4491	1118	50.008	0.500 24 . 63
MOTA	937	СВ	BGLN	126	6.525	27.417	3751	-881 -2407 462
ANISOU	937	CB	BGLN	126	1695	1137	48.018	0.500 13.36
MOTA	938	CG	BGLN	126	6.604	27.750	2245	602 -114 - 255
ANISOU	938	CG	BGLN	126	2537	27.750	49.497	0.500 18.28
MOTA	939	CD	BGLN	126	5.442	27.237	2153	-68 -176 - 105
ANISOU	939	CD	BGLN	126	2.442	2573	50.319	0.500 18.42
ATOM	940		BGLN	126	5.605	26.442	2198	344 -159 1 0 6
ANISOU	940	OE1	BGLN	126	3280	3517	51.242	0.500 25.36
ATOM	941	NE2	BGLN	126	4.231	27.685	2828	-100 -223 9 5 3
ANISOU	941	NE2	BGLN	126	2427	2669	50.003	
ATOM	942	C	GLN	126	7.860		4413	1004 -83 -298
ANISOU		Č	GLN		1506	27.448 1434	45.861	1.000 12.95
MOTA	943	ŏ	GLN		8.859	26.721	1979	307 -372 - 366
ANISOU		Ö	GLN	126	1461	1142	45.748	1.000 11.66
ATOM	944	N	TYR		6.960	27.578	1827	182 -85 159
ANISOU		N	TYR	127	1400	1276	44.868	1.000 11.61
ATOM	945	CA	TYR	127	7.152		1735	146 -168 - 10
ANISOU		CA	TYR		1469	26.869	43.585	1.000 11.21
ATOM	946	CB	TYR	127	5.901	1242	1550	-92 -40 192
	-			/	J. 901	26.940	42.724	1.000 11.82

- 121 -CB TYR ANISOU 946 CG TYR 947 MOTA CG TYR ANISOU 947 CD1 TYR 948 MOTA ANISOU 948 CD1 TYR 127 1030 -100 3 CE1 TYR 127 6.406 24.153 40.115 1.000 11.47 CE1 TYR 127 1164 1167 2027 -51 -53 2 1 949 MOTA ATOM 949 CE1 TYR 127 1164 1167 2027 -51 -53 2 1 ATOM 950 CD2 TYR 127 4.871 26.410 40.500 1.000 11.98 ANISOU 950 CD2 TYR 127 4.715 25.655 39.357 1.000 11.37 ANISOU 951 CE2 TYR 127 1539 1118 1665 140 -68 -73 ATOM 952 CZ TYR 127 5.494 24.508 39.163 1.000 11.02 ANISOU 952 CZ TYR 127 1202 1226 1760 91 48 -125 ATOM 953 OH TYR 127 5.379 23.720 38.030 1.000 11.57 ANISOU 953 OH TYR 127 5.379 23.720 38.030 1.000 11.57 ANISOU 953 OH TYR 127 1547 1138 1712 94 177 -34 ATOM 954 C TYR 127 1547 1138 1712 94 177 -34 ATOM 955 O TYR 127 1296 989 1830 230 -43 3 7 8 ATOM 955 O TYR 127 1296 989 1830 230 -43 3 7 8 ATOM 955 O TYR 127 1296 989 1830 230 -43 3 7 8 ATOM 955 O TYR 127 1292 1232 1603 164 -237 - 4 2 ATOM 956 N THR 128 8.565 28.716 42.865 1.000 10.98 ANISOU 956 N THR 128 1554 976 1642 212 -9 5 5 7 ATOM 957 CA THR 128 1554 976 1642 212 -9 5 5 7 ATOM 958 CB THR 128 1686 1125 1673 -47 -169 3 8 6 ANISOU 958 CB THR 128 1686 1125 1673 -47 -169 3 8 6 ANISOU 958 CB THR 128 1873 1074 1864 -52 -233 5 2 1 ATOM 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 9 ANISOU 949 959 OG1 THR 128 2223 1597 2542 124 -457 9 9 8 960 CG2 THR 128 10.878 31.510 41.893 1.000 16.54 ANISOU 959 OG1 THR 128 2223 ATOM ANISOU 960 CG2 THR 128 1871 778 3635 262 655 1 3 8 MOTA 961 C THR 128 11.040 28.828 42.964 1.000 11.26 ATOM 961 C THR 128 11.040 28.828 42.964 1.000 11.26 ANISOU 961 C THR 128 1562 980 1738 -71 -162 148 ATOM 962 O THR 128 11.995 28.458 42.258 1.000 12.16 ANISOU 962 O THR 128 1769 1092 1758 17 26 2 7 9 ATOM 963 N ALA 129 11.083 28.802 44.300 1.000 10.39 ANISOU 963 N ALA 129 1183 1001 1763 70 -118 147 ATOM 964 CA ALA 129 12.273 28.386 45.037 1.000 10.59 ANISOU 964 CA ALA 129 12.273 28.386 45.037 1.000 10.59 ANISOU 965 CB ALA 129 12.113 28.603 46.536 1.000 12.46 ANISOU 965 CB ALA 129 2113 851 1769 82 -218 5 77 ATOM 966 C ALA 129 12.575 26.906 44.802 1.000 11.35 ANISOU 966 C ALA 129 1258 883 2170 -16 -141 410 ATOM 967 O ALA 129 13.738 26.485 44.641 1.000 10.93 ANISOU 967 O ALA 129 1202 1157 1796 -36 -213 1 ANISOU 967 O ALA 129 1202 1157 1796 -36 -213 1 2 1 ATOM 968 N SER 130 11.519 26.086 44.750 1.000 12.27 ANISOU 968 N SER 130 1280 984 2398 -65 -1 - 2 4 969 CA SER 130 11.682 24.650 44.512 1.000 10.89 ATOM ANISOU 969 CA SER 130 1623 876 1638 -85 44 3 7 0 970 CB ASER 130 10.342 23.940 44.716 0.500 10.08 ANISOU 970 CB ASER 130 1432 603 1793 213 247 4 1 3 ATOM 971 OG ASER 130 9.771 24.063 46.006 0.500 9.12 ANISOU 971 OG ASER 130 1021 651 1792 91 1 -143 972 CB BSER 130 10.364 23.919 44.765 0.500 10.60 ATOM ANISOU 972 CB BSER 130 1687 822 1521 -45 318 1 5 8
ATOM 973 OG BSER 130 9.418 24.098 43.734 0.500 16.22
ANISOU 973 OG BSER 130 1717 1289 3156 137 -525 3 4 8
ATOM 974 C SER 130 12.214 24.373 43.110 1.000 10.53 С SER 130 1586 733 1684 -166 210 4 8 4 SER 130 13.137 23.532 42.942 1.000 11.17 ANISOU 974 ATOM 975 O SER 130 13.137 23.532 42.942 1.000 11.17 ANISOU 975 O SER 130 1385 1012 1849 -151 -95 140 ATOM 976 N ARG 131 11.680 25.044 42.079 1.000 10.46 ANISOU 976 N ARG 131 1578 861 1534 -87 -66 9 9

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ATOM	977	CA	ARG		12.260	24.839	40 742	1.000 10.60
ANISO ATOM		CA	ARG		1480	1110	1438	61 -288 2
ANISO	978	CB	ARG	131	11.426	25.553	39.679	1.000 12.99
ATOM	979	CB CG	ARG		1893	1369	1673	63 - 525 276
ANISO		CG	ARG	131	10.003	25.065	39.431	1.000 13.64
ATOM	980	CD	ARG		1707	1735	1742	335 -559 - 86
ANISO		CD	ARG ARG		9.349	25.669	38.206	1.000 17.71
ATOM	981	NE	ARG	131	. 2078 . 9.453	1973	2677	81 - 983 701
ANISO		NE	ARG	131	2716	27.113	38.015	
ATOM	982	CZ	ARG	131	8.629	2034	2757	-25 -525 7 1 3
ANISO	J 982	CZ	ARG	131	3688	28.004 1878	38.568	
ATOM	983		ARG		7.631	27.634	2503	-8 -128 647
ANISOU		NHI	ARG	131	2792	3142	39.366 2166	
ATOM	984	NH2	ARG		8.771	29.310	38.361	-486 -667 5 7
ANISOU			ARG	131	4649	1822	4103	1.000 27.83 -90 -422 5 6 1
MOTA	985	C	ARG	131	13.714	25.323	40.688	-90 -422 5 6 1 1.000 10.42
ANISOU ATOM		C	ARG		1542	1078	1339	50 -103 1
ANISOU	986	0	ARG	131		24.683	40.080	1.000 10.94
ATOM	987	N O	ARG	131	1544	1105	1506	177 -134 4 2
ANISOU		N	ALA	132		26.438	41.343	1.000 10.97
ATOM	988	CA	ALA ALA	132		1129	1563	74 - 364 - 45
ANISOU		CA	ALA	132	15.379 1539	26.983	41.343	1.000 11.10
MOTA	989	СВ	ALA		15.429	944 17		-102 9 7
ANISOU	989	CB	ALA	132	1711	28.344 1171	42.048	1.000 12.82
ATOM	990	С	ALA		16.393	26.045	1987	-48 -248 - 198
ANISOU		С	ALA	132	1085	1107	41.995 2197	1.000 11.55
ATOM	991	0	ALA		17.481	25.832	41.432	-197 305 745
ANISOU		0	ALA	132	1081	1809	1599	1.000 11.81 -204 17 - 9
ATOM	992	N	VAL	133	16.061	25.490	43.175	-204 17 - 9 1.000 11.16
ANISOU ATOM		N	VAL		1260	1356	1623	-148 51 3 5 0
ANISOU	993	CA	VAL	133	17.011	24.587	43.840	1.000 11.62
ATOM	994	CA	VAL	133	1505	1529	1380	-69 -297 8 9
ANISOU		CB CB	VAL	133	16.738	24.418	45.344	1.000 12.14
ATOM	995		VAL VAL		1376	1674	1564	-74 -25 364
ANISOU		CGI	VAL		15.550	23.501	45.608	1.000 14.96
ATOM	996	CG2	VAL		1705 17.981	2316	1662	-706 8 -357
ANISOU		CG2	VAL	133	17.981	23.864 2340	46.033	1.000 15.63
ATOM	997	С	VAL		17.079	23.268	1845	-341 -677 5 5 1
ANISOU	997	С	VAL	133	1376		43.065	1.000 11.71
ATOM	998	0	VAL	133	18.198	22.733	42.925	-24 -425 1 6 9
ANISOU		0	VAL	133	1391	1453	1545	1.000 11.55 -4 -116 3 9 8
ATOM	999	N	ALA	134	15.982	22.758	42.480	-4 -116 398 1.00012.87
ANISOU		N	ALA	134	1399	1517	1973	28 -334 - 228
ATOM ANISOU	1000	CA	ALA	134	16.084	21.557	41.621	1.000 10.57
ATOM	1000	CA	ALA		1106	1220	1691	153 -298 9 6
ANISOU	1001	CB	ALA	134	14.699	21.096	41.186	1.000 12.20
ATOM	1001		ALA	134	1254	1589	1794	35 - 303 - 127
ANISOU	1002	Č	ALA ALA	134	16.968	21.797	40.399	1.000 12.58
ATOM	1003	0	ALA	134	1393		1987	272 -4 2 7 7
ANISOU	1003	ŏ	ALA	134	17.712 1254	20.924	39.970	1.000 11.01
ATOM	1004	N	ARG	135	16.908	1358	1574	83 - 268 2 6
ANISOU	1004	N	ARG	135	1517	22.995 1230	39.809	1.000 12.03
ATOM	1005	CA	ARG	135	17.773	23.353	1824	-62 -327 8 7
ANISOU	1005	CA	ARG	135	1854	1158	38.676 2015	1.000 13.23
ATOM	1006	CB	ARG		17.393	24.734	38.170	-270 -209 1 6 1
ANISOU	1006	CB	ARG	135	2203	1339	1994	1.000 14.57 -45 -541 2.2.2
ATOM	1007	CG	ARG	135	17.753		36.797	-45 -541 2 2 2 1.000 19.22



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ANISOU	1007	CG	ARG	135	4204	1120	1980	-490 -433 1 5 0
ATOM	1008	CD	ARG	135	17.237	26.563	36.471	1.000 22.14
ANISOU	1008	CD	ARG	135		1500	2868	-159 315 822
ATOM	1009		ARG	135	15.831	26.607		1.000 22.66
ANISOU	1009	ΝE	ARG	135	4239	1404	2965	-94 47 2 5 7
ATOM	1010		ARG	135	14.802	27.184	36.684	1.000 21.69
ANISOU	1010	CZ	ARG	135		1906	2333	92 - 506 6 4
ATOM	1011		ARG		14.917	27.843	37.833	1.000 22.26
ANISOU				135		2532	1812	460 -833 3 4 1
ATOM	1012				13.582	27.113	36.149	1.000 22.31
ANISOU	1012	NH2	ARG	135		2243	2234	-544 -419 8
ATOM	1013		ARG		19.251	23.275	39.057	1.000 12.70
ANISOU			ARG	135	1742	1264	1821	-119 -16 430
ATOM	1014		ARG	135	20.069	22.818	38.238	1.000 14.67
ANISOU	1014	0	ARG	135		1529	1910	19 169 3 9 1
ATOM	1015		GLU	136	19.572	23.712	40.266	1.000 12.15
ANISOU	1015	N	GLU	136	1423	1372	1820	-36 70 4 3 0
ATOM	1016		GLU	136	20.960	23.630	40.763	1.000 14.52
ANISOU			GLU	136		1701	2194	-90 -197 3 7 1
ATOM	1017	СВ	GLU	136	21.212	24.513	41.981	1.000 15.59
ANISOU			GLÜ		1502	1781	2642	14 -231 1 1
ATOM	1018		GLU		21.064	26.020		1.000 18.01
ANISOU			GLU	136	2010	1762	3071	-232 -153 1 2 6
ATOM	1019		GLU	136	21.798	26.484	40.537	1.000 20.18
ANISOU	1019	CD	GLU	136	2071	2079	3519	-308 89 3 6 9
ATOM	1020	OE1	GLU		22.987	26.148	40.394	1.000 24.64
ANISOU	1020	OE1	GLU	136	2060	2937	4364	-262 338 615
ATOM	1021	OE2	GLU		21.195	27.150	39.670	1.000 24.19
ANISOU	1021	OE2	GLU	136	2479	2327	4385	-381 317 1426
ATOM	1022	С	GLU	136	21.364	22.186	41.076	1.000 14.00
ANISOU	1022	С	GLU	136	1338	1619	2361	-112 -442 2 2 3
MOTA	1023		GLU	136	22.508	21.781	40.833	1.000 13.86
ANISOU	1023	0	GLU	136	1366	1890	2009	-100 -287 3 2 9
MOTA	1024	N	VAL	137	20.472	21.338	41.580	1.000 11.78
ANISOU	1024	N	VAL		1309	1451	1715	148 -223 8 5
MOTA	1025		VAL		20.753	19.896	41.771	1.000 12.49
ANISOU	1025	CA	VAL		1369	1522	1853	240 -69 289
MOTA	1026		VAL		19.560	19.165	42.429	1.000 12.41
ANISOU			VAL	137	1422	1424	1869	-67 -85 -204
MOTA			VAL		19.728	17.634		1.000 12.55
ANISOU					1371	1508	1892	182 185 111
MOTA			VAL		19.355	19.607	43.852	1.000 11.35
ANISOU			VAL			1281		182 -254 2 8 8
MOTA	1029		VAL		21.100			1.000 12.48
ANISOU			VAL		1202	1428	2113	150 -16 8 5
ATOM	1030		VAL		22.057	18.462		1.000 13.03
ANISOU			VAL		1021	1683		149 1 146
ATOM	1031		LEU		20.309	19.562	39.401	1.000 10.28
ANISOU			LEU		1198			5 158 2 2 6
ATOM	1032		LEU		20.571	19.029		1.000 12.48
ANISOU			LEU		1312	1408		110 273 - 52
MOTA	1033		LEU		19.398	19.358		1.000 11.81
ANISOU			LEU		1260	1586		
MOTA	1034		LEU		18.036	18.726		1.000 10.77
ANISOU			LEU		1391	1397		
MOTA			LEU		16.916	19.324		
ANISO					1416	1587		
ATOM			LEU		18.052	17.207		
ANISO					1986	1390	2065	-79 296 370
MOTA	103		LEU		21.903	19.525		
ANISO	J 103'	7 C	LEU	138	1305	2026	1840	-65 174 5

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ATOM ANISC ATOM	0 103 103 103 104 104 104 104 104 104 104 104 104 104	9900112233445557788 NN CCCCCCOONN CCCCCCCOONN CAABB 1122233445557788 NN CCCCCCCOONN CCCCCCCCOONN CCA	ARGGGGGGGGGAAAAAAAAAAAAAAAAAAAAAAAAAAA	138 139 139 139 139 139 139 139 139 139 139	24.207 1238 22.946 1249 24.167 1394 25.423 1732 25.432 1991 25.474 2127 25.611	220.46 21.71 20.46 21.71 20.46 21.94 21.01 2	2313 37.61 37.00 37.775 2000 37.775 37.166 2688 37.206 38.30 36.237 36.11 37.21 37.22 38.849 37.22 38.88 39.09 2151 39.85 39.39	1 1.000 13.26 -155 219 317 1.000 14.71 -27 502 447 1.000 15.16 -158 324 1 1 6 1.000 18.15 18 612 3 3 9 1.000 19.67 -196 186 2 5 2 1.000 28.66 -2305 882 -5 6 3 1.000 39.58 -3273 119 -3 0 6 1.000 47.91 -2157 -1331 -7 0 8 1.000 45.42 -882 -2118 -1 2 3 8 1.000 64.33 93 -2965 -9 8 0 1.000 32.62 -2746 590 1 6 7 1.000 14.85 -517 -26 -4 6 1.000 15.80 09 -9 -4 0 1 1.000 19.36 243 -435 -4 8 0 1.000 16.86 12 -186 -4 5 8 1.000 18.90 -21 60 145 1.000 17.53 -528 218 -1 0 8 1.000 15.59 -192 -95 2 9 1 1.000 14.77 155 282 3 0 1 1.000 14.77 155 282 3 0 1 1.000 15.59 -192 -95 2 9 1 1.000 14.77 155 282 3 0 1 1.000 15.59 -192 -95 2 9 1 1.000 17.55 282 3 0 1 1.000 17.55 282 3 0 1 1.000 17.55 283 3 3 2 5 1.000 17.55 237 555 2 4 9 1.000 17.74 303 260 5 0 1 1.000 17.32
ANISOU ATOM ANISOU ATOM	1060 1060 1061 1061 1062	C C O N	THR THR THR THR	141 141 141 141	1394 25.423 1732 25.432 1991	2077 16.374 2046 15.235 2104	2160 37.257 2343 36.778 2573	135 -47 177 1.000 16.11 303 583 325 1.000 17.55 237 555 249
ATOM ANISOU ATOM ANISOU ATOM	1063 1063 1064 1064 1065	N CA CA C C	GLY GLY GLY GLY GLY	142 1 142 1 142 1 142 1	2127 25.611 1642 24.426	2197 17.263 2494 16.556 1893	2416 34.987 2447 34.358 2710	303 260 5 0 1 1.000 17.32 -160 453 5 1 7 1.000 16.37 261 472 4 2
ANISOU ATOM ANISOU ATOM ANISOU ATOM	1065 1066 1066 1067	O N N CA CA	GLY THR THR THR THR	142 2 143 2 143 1 143 2 143 1	2243 23.232 1531 22.049	2558 16.738 1429 16.003	2201 34.907 2356 34.472 2223	1.000 18.43 57 798 1 6 3 1.000 13.99 83 430 3 5 0 1.000 14.69 8 342 9 3 1.000 15.52
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ANISOU	1068	СВ	THR	143	1457	1653	2785	55 419 5 2 9
ATOM	1069				22.037	14.784		1.000 - £4, 63
ANISOU					1296	1792	2471	52 434 3 6 9
ATOM	1070				20.044	14.738	35.231	1.000 14.24
ANISOU					1761	1981	1669	
ATOM	1070							3 379 1 9 2
			THR		21.135	16.785		1.000 13.96
ANISOU			THR		1553	1708	2044	128 479 -131
ATOM		0	THR		20.642	17.828	33.923	1.000 15.65
ANISOU			THR		2374	1580	1995	315 486 5 5
ATOM	1073		GLU		20.928		32.322	1.000 15.32
ANISOU			GLU		1734	1904	2184	-156 260 -271
ATOM	1074		GLU		19.917	16.693	31.362	1.000 17.30
ANISOU			GLU		1686	2470	2417	-377 152 106
ATOM	1075		GLU	144	18.774	15.693	31.292	1.000 16.84
ANISOU	1075	С	GLU	144	1633	2380	2386	-298 313 -242
MOTA	1076	0	GLU	144	18.922	14.631	30.680	1.000 16.71
ANISOU	1076	0	GLU		1470	2057	2821	-43 610 5 8
ATOM	1077		GLU		20.539	16.856	29.970	1.000 21.91
ANISOU			GLU		2747	3417	2162	-1508 31 - 8
ATOM	1078		GLU		19.568	17.063	28.825	1.000 37.93
ANISOU			GLU		6652	4374	3385	-2057 -2082 1767
ATOM	1079		GLU		19.293	18.507		
ANISOU			GLU		7869	4258		
ATOM	1080				19.602	19.365	4419	-2497 -2259 2129
ANISOU								1.000 51.81
					9843	4613	5230	-3180 -832 1126
ATOM	1081				18.766	18.798	27.367	1.000 40.12
ANISOU					5551	6029	3662	-285 -115 2 6 6 0
ATOM	1082		PRO		17.620	15.959	31.908	1.000 14.29
ANISOU			PRO		1634	1364	2432	-4 208 265
ATOM	1083		PRO		17.256	17.136	32.718	1.000 14.14
ANISOU			PRO		1735	1778	1859	-55 32 1 6 7
ATOM	1084		PRO	145		15.000	31.807	
ANISOU			PRO		1484	1391	2337	66 173 4 6 6
ATOM	1085	CB	PRO	145	15.406	15.701	32.606	1.000 14.20
ANISOU			PRO	145	1459	1636	2302	161 -41 289
ATOM	1086	CG	PRO	145	16.132	16.608	33.561	1.000 14.43
ANISOU	1086	CG	PRO	145	1796	2007	1679	-23 -42 449
ATOM	1087	С	PRO	145	16.076	14.794	30.372	1.000 15.18
ANISOU	1087	С	PRO	145	1745	1665	2359	-192 231 287
MOTA	1088		PRO		16.178	15.685	29.509	1.000 15.40
ANISOU			PRO		2430	1511	1910	-85 613 -15
ATOM	1089		ASP		15.544	13.613	30.070	
ANISOU			ASP		2019	1611	2367	
ATOM	1090		ASP		14.918	13.366	28.773	1.000 16.74
ANISOU			ASP		2095	1759	2506	-348 575 - 77
ATOM	1091		ASP		14.300	11.966	28.727	1.000 18.99
ANISOU			ASP		2508	1729	2977	-323 780 -439
ATOM	1092		ASP		13.504	11.784		
							27.444	
ANISOU			ASP		4012	2450	3813	-720 <b>-</b> 229 - 805
ATOM	1093				12.295	12.121	27.409	1.000 38.65
ANISOU					3943	4889	5852	-595 -1282 - 323
ATOM			ASP		14.091	11.311	26.466	1.000 39.95
ANISOU					6913	5052	3214	160 -1182
ATOM	1095		ASP		13.860	14.441	28.552	
ANISOU			ASP		2461	1904	1961	-128 580 -40
MOTA	1096		ASP		13.041	14.605	29.457	1.000 15.67
ANISOU			ASP		2110	1935	1908	-334 381 -420
MOTA	1097		GLY	147	13.871	15.149	27.429	
ANISOU			$\mathtt{GLY}$		3484	2416	1927	-26 419 129
ATOM	1098	CA	GLY	147	12.903	16.212	27.155	1.000 18.06
ANISOU	1098	CA	GLY		2771	2451	1638	-382 98 9 3
								-

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ATOM 1099 C	GLY 147 1			
ANISOU 1099 C	GLY 147 2			
ATOM 1100 O				$-524 - \overline{143}  527$
ANISOU 1100 O	GLY 147 2		.570 27.282 16 1687	
ATOM 1101 N	GLY 148 1		.634 28.316	7-413 -72 389
ANISOU 1101 N	GLY 148 2	936 15	06 1772	
ATOM 1102 CA	GLY 148 1		.889 28.747	-157 142 8 8
ANISOU 1102 CA	GLY 148 2	723 12	79 1829	
ATOM 1103 C	GLY 148 1		.339 30.144	55 450 - 26
ANISOU 1103 C	GLY 148 2	231 14		
ATOM 1104 O	GLY 148 1		.930 30.771	-93 -62 407 1.000 13.79
ANISOU 1104 O		301 13 <sup>.</sup>	76 1561	
ATOM 1105 N	VAL 149 1	5.604 20	.224 30.718	-164 88 3 2 3 1.000 12.81
ANISOU 1105 N ATOM 1106 CA	VAL 149 1	815 13	66 1686	155 -31 238
ATOM 1106 CA ANISOU 1106 CA	VAL 149 1	5.388 20	.724 32.079	1.000 11.81
ATOM 1106 CA	VAL 149 1:	333 139	90 1765	54 -92 1 2 9
ATOM 1107 CB ANISOU 1107 CB	VAL 149 16		.636 32.480	1.000 11.97
ATOM 1107 CB	VAL 149 1:		96 1717	-100 246 124
ANISOU 1108 CG1			.336 33.802	1.000 15.26
ATOM 1109 CG2			22 1936	-195 55 - 223
ANISOU 1109 CG2			794 32.538	1.000 17.21
ATOM 1110 C				45 102 - 103
ANISOU 1110 C	VAL 149 14 VAL 149 11		482 32.280	1.000 11.32
ATOM 1111 O				-78 131 479
ANISOU 1111 O	VAL 149 13 VAL 149 16		218 33.253	1.000 12.35
ATOM 1112 N	GLU 150 13			-71 229 167
ANISOU 1112 N	GLU 150 13		463 31.460	1.000 11.96
ATOM 1113 CA	GLU 150 13			29 -36 4 2 0
ANISOU 1113 CA	GLU 150 16	1392 23. 135	286 31.815	1.000 10.90
ATOM 1114 CB	GLU 150 12			118 0 4 0 5
ANISOU 1114 CB	GLU 150 25	30 147		1.000 17.60
ATOM 1115 CG	GLU 150 13			181 -161 9 0 7
ANISOU 1115 CG	GLU 150 27		3246 246	1.000 17.86
ATOM 1116 CD	GLU 150 13			
ANISOU 1116 CD	GLU 150 30	18 135	3 3027	1.000 19.47 -97 -84 662
ATOM 1117 OE1	GLU 150 12	.951 26.	005 33.475	-97 -84 662 1.000 18.21
ANISOU 1117 OE1		35 151		-178 -321 5 3 6
ATOM 1118 OE2		.109 26.		1.000 22.59
ANISOU 1118 OE2 ATOM 1119 C		93 166	4 3927	-38 -150 2 8 4
	GLU 150 11		533 31.705	1.000 12 22
3	GLU 150 14		0 1676	235 147 - 5
33770000	GLU 150 10	.341 22.	757 32.530	1.000 13.44
3	GLU 150 17			315 470 288
11170000	ALA 151 11 ALA 151 17			1.000 11.88
3 0000				94 45 253
11770000			844 30.698	1.000 13.82
3 00 00 00 00 00	ALA 151 17 ALA 151 9.			-100 -413 3 9 6
33770000	ALA 151 14			1.000 14.89
3 7 6 4 4 4 4	ALA 151 9.			22 - 269 - 35
ANISOU 1124 C	ALA 151 14			1.000 12.71
ATOM 1125 O	ALA 151 8.			93 41 4 2 4
ANISOU 1125 O	ALA 151 15	655 19. 35 211		1.000 14.69
ATOM 1126 N	PHE 152 10	.925 19.		-242 204 -108
ANISOU 1126 N	PHE 152 15	98 125		1.000 11.73
ATOM 1127 CA	PHE 152 10	.890 18.		120 9 271
ANISOU 1127 CA	PHE 152 14	44 106	554 33.602 1 1526	1.000 10.61
	PHE 152 12	.293 17.		-33 34 1 6 0 1 000 10 33
	PHE 152 13:	17 113	2 1437	1.000 10.23 -144 207 410
ATOM 1129 CG	PHE 152 12			1.000 10.36
	•	•		2.000 10.30

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ANISOU	1129	CG	PHE	152	1388	1149	1399	-34 147 276
MOTA	1130	CD1	PHE	152	12.036	15.896	35.229	1.000-l-II24
ANISOU				152		1047	1743	114 -103 5 6 6
ATOM	1131	CD2	PHE	152	13.229	17.701	36.154	1000 11.21
ANISOU					1489	1449	1319	85 174 151
ATOM	1132				12.252	15.163	36.380	1.000 10.80
ANISOU					1400	1234	1467	249 -111 3 7 3
ATOM	1133				13.431	16.992	37.341	1.000 11.82
ANISOU					1709	1622	1160	-276 414 250
ATOM	1134		PHE		12.932	15.717	37.457	1.000 11.97
ANISOU			PHE		1651	1604	1293	-255 296 170
ATOM	1135		PHE		10.430	19.292	34.858	1.000 12.24
ANISOU			PHE		1754	1168	1730	-10 339 8 4
ATOM	1136		PHE		9.728	18.729	35.726	1.000 11.49
ANISOU			PHE		1672	1142	1550	200 109 277
ATOM	1137		LEU		10.809	20.575	34.997	1.000 11.86
ANISOU	1137	N	LEU	153	2030	1236	1240	-673156
MOTA	1138	CA	LEU	153	10.532	21.386	36.155	1.000 11.99
ANISOU	1138	CA	LEU	153	1890	1229	1437	-165 307 8 5
MOTA	1139	CB	LEU	153	11.654	22.420		1.000 12.81
ANISOU	1139	CB	LEU	153	1691	1381	1794	-72 97 - 40
ATOM	1140		LEU		13.059	21.910		1.000 12.87
ANISOU			LEU		1762	1645	1483	146 269 6 4
ATOM	1141				14.027	23.081	36.611	1.000 15.99
ANISOU					1609	2006	2462	-49 450 -431
MOTA	1142				13.185	21.158		1.000 19.37
ANISOU					3091	2462	1806	809 275 540
ATOM	1143		LEU		9.179	22.084		1.000 12.96
ANISOU			LEU		1728	1253	1943	-336 360 - 43
ATOM	1144		LEU		8.709	22.506	37.193	1.000 13.24
ANISOU			LEU		1617	1302	2109	-443 481 -182
ATOM	1145		ASP		8.568	22.203	34.955	1.000 13.29 60 517 280
ANISOU			ASP		1643	1457	1951	
ATOM	1146		ASP		7.195	22.671	34.764	313 631 683
ANISOU ATOM	1140		ASP ASP		1862 6.995	1255 23.269	2280 33.373	1.000 18.38
ANISOU			ASP		2091	23.269	2738	328 728 1475
ANISOU	1148		ASP		5.534	23.367	32.929	
ANISOU			ASP		2323	3543	2855	676 430 1501
ATOM	1149				4.685	23.607		-
ANISOU			ASP		2164	23.667	33.820	895 478 1144
ATOM			ASP		5.168	23.254	31.702	
ANISOU					2989	3146	3110	228 48 1 1 2 8
ATOM	1151		ASP	154	6.294	21.455	34.985	
ANISOU			ASP		1594	1403	1265	123 147 410
ATOM	1152		ASP		6.043	20.729	34.015	
ANISOU			ASP		2143	1728	1186	427 219 1 7 0
ATOM	1153		CYS		5.891	21.220	36.233	
ANISOU			CYS	155		1098	1243	-76 186 2 7
ATOM	1154		CYS		5.446	19.881	36.627	
ANISOU			CYS		1294	1168	1115	-13 154 172
ATOM	1155		CYS		6.635	19.171		
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- 128 -1160 CA GLU 156 2.778 MOTA 18.787 39.173 1.000 9.04 ANISOU 1160 CA GLU 156 998 1160 1278 -76 -37-2,36 ATOM 1161 CB GLU 156 2.300 17.391 38.772 1.000 11.63
ANISOU 1161 CB GLU 156 1187 1348 1885 -67 -135 ANISOU 1162 CG GLU 156 1.841 17.282 37.326 1.000 14.29
ANISOU 1162 CG GLU 156 1741 1640 2049 -628 -507 5
ANISOU 1163 CD GLU 156 0.502 17.949 37.039 1.000 17.90
ANISOU 1163 CD GLU 156 1772 2692 2336 -365 -686 1 1885 --67 -135 - 190 -628 -507 5 0 -365 -686 1 3 7 1164 OE1 GLU 156 -0.220 18.241 38.024 1.000 19.17 MOTA ANISOU 1164 OE1 GLU 156 1429 2973 2884 -632 -270 2 5 3 1165 OE2 GLU 156 0.136 ATOM ATOM 1165 OE2 GLU 156 0.136 18.198 35.858 1.000 22.03 ANISOU 1165 OE2 GLU 156 2449 3269 2653 -243 -721 9 2653 -243 -721 9 2 4 1166 C 156 2.961 18.942 40.677 1.000 9.21 ATOM GLU 156 1166 1135 1197 -26 239 1 8 3 156 2.828 17.997 41.476 1.000 11.22 ANISOU 1166 C GLU 1167 o ATOM GLU ANISOU 1167 O 156 1631 1199 1434 103 162 4 157 3.337 20.158 41.118 1.000 10.29 GLU 103 162 431 MOTA 1168 N PRO 

 157 3.337
 20.158
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 1.000 10.29

 157 1329
 1201
 1381
 -109 21 123

 157 3.527
 21.407
 40.359
 1.000 10.17

 157 1381
 1093
 1391
 -40
 -30 2 1

 157 3.618
 20.363
 42.553
 1.000 10.28

 157 1160
 1354
 1391
 -12
 -61 6 4

 157 4.173
 21.805
 42.590
 1.000 12.44

 157 1832
 1567
 1330
 -397 20 5 8

 157 3.475
 22.471
 41.429
 1.000 10.44

 157 1469
 1259
 1237
 -388 166 - 1

 ANISOU 1168 N PRO 1169 CD PRO ATOM ANISOU 1169 CD PRO 1170 CA PRO ATOM ANISOU 1170 CA PRO MOTA 1171 CB PRO ANISOU 1171 CB PRO 1172 CG PRO MOTA ANISOU 1172 CG PRO ATOM 1173 C ANISOU 1173 C MOTA 1174 O PRO 157 11.247
PRO 157 1157
1742
1426
-93
-64
3
3
LEU 158 2.561
19.988
44.742
1.000
9.91
LEU 158 1011
1308
1447
-86
-53
151
LEU 158 1319
1461
1344
-387
-2
-3
LEU 158 1.152
18.482
46.078
1.000
11.03 ANISOU 1174 O ATOM 1175 N ANISOU 1175 N 1176 CA MOTA ANISOU 1176 CA ATOM 1177 CB ANISOU 1177 CB ANISOU 1177 CB LEU 158 1.152 18.482 46.078 1.000 11.03
ATOM 1178 CG LEU 158 0.111 18.239 47.155 1.000 12.01
ANISOU 1178 CG LEU 158 1271 1497 1795 -303 241 1 28
ATOM 1179 CD1 LEU 158 -1.212 18.826 46.736 1.000 16.21
ANISOU 1179 CD1 LEU 158 1224 2249 2685 -111 41 -239
ATOM 1180 CD2 LEU 158 -0.086 16.736 47.397 1.000 17.17
ANISOU 1180 CD2 LEU 158 2656 1542 2325 -254 1273 1 7 4 ATOM 1180 CD2 LEU 158 -0.086 16.736 47.397 1.000 17.17

ANISOU 1180 CD2 LEU 158 2656 1542 2325 -254 1273 1 7 4

ATOM 1181 C LEU 158 1.997 20.626 47.048 1.000 11.22

ANISOU 1181 C LEU 158 1496 1366 1402 110 -304 5

ATOM 1182 O LEU 158 3.056 20.201 47.539 1.000 11.28

ATOM 1183 N LEU 159 1.234 21.599 47.548 1.000 10.86

ANISOU 1183 N LEU 159 1103 1744 1278 68 -180 - 70

ANISOU 1184 CA LEU 159 1.540 22.278 48.797 1.000 11.62

ATOM 1185 CB LEU 159 1247 1761 1407 -59 -68 -180

ATOM 1185 CB LEU 159 1.494 23.802 48.640 1.000 12.44

ANISOU 1185 CB LEU 159 1633 24.635 49.934 1.000 12.83

ANISOU 1186 CG LEU 159 1.633 24.635 49.934 1.000 12.83

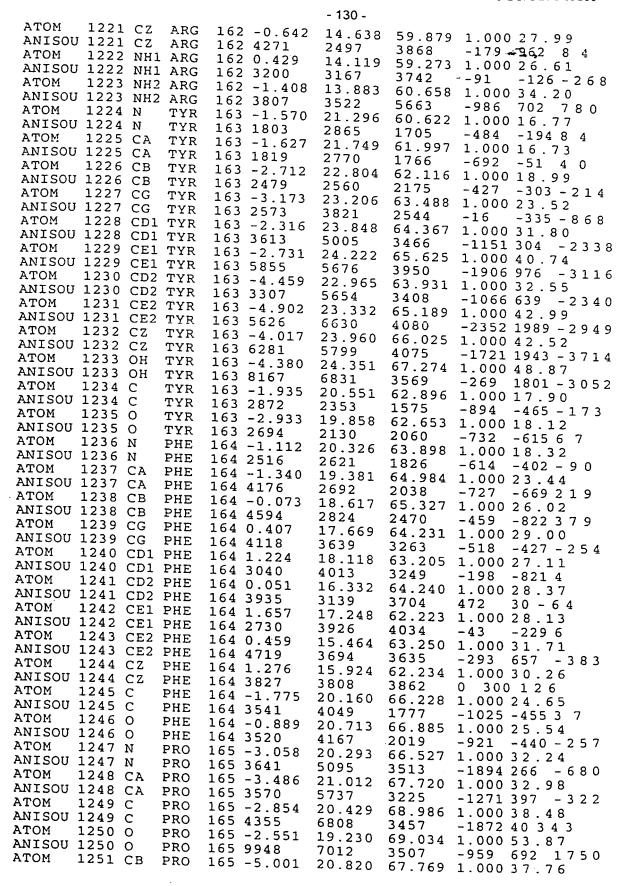
ANISOU 1187 CD1 LEU 159 2.947 24.435 50.651 1.000 14.28

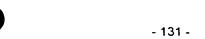
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ATOM 1188 CD2 LEU 159 1.442 26.134 49.640 1.000 13.33 -59 -68 -180 246 -54 -215 159 1.442 26.134 49.640 1.000 13.33 ANISOU 1188 CD2 LEU 159 1802 159 1802 1721 1543 87 -87 - 20 159 0.537 21.846 49.868 1.000 11.24 ATOM 1189 C LEU ANISOU 1189 C LEU 159 1393 1474 1404 -174 -9 -271159 -0.665 21.940 49.620 1.000 13.70 ATOM 1190 O LEU



ANISOU ATOM ANISOU ATOM	1191	N N	LEU ARG ARG ARG	160 160	1354 1.013 1737 0.158	2395 21.385 2569 21.030	1457 51.010 1239	-328 34 - 269 1.000-T4, 59 -390 -128 - 224
ANISOU	1192	CA	ARG	160	1265	2631	1402	-1.000 13.94 157 -137 9 2
ATOM	1193		ARG		0.161	19.528	52.343	1.000 18.20
ANISOU ATOM	1193		ARG ARG		1932 -0.423	2645 18.661	2338 51.252	-301 32 1 9 3
ANISOU			ARG		3451	2902	31.252	1.000 25.12 -653 -787 2 3
MOTA	1195		ARG	160	-0.765	17.301	51.831	1.000 31.98
ANISOU ATOM	1195		ARG		4825	3598	3729	-1994 -905 3 2 1
ANISOU			ARG ARG		-1.28 <u>4</u> 3392	16.322 2957	50.896 3587	1.000 26.15 -739 -1056 310
ATOM	1197	CZ	ARG		-0.970	15.044	50.779	1.000 25.30
ANISOU			ARG		3195	3390	3028	94 - 785 295
ATOM ANISOU	1198 1198				-0.063 3654	14.433 4142	51.552 4080	1.000 31.26
ATOM	1199	NH2	ARG		-1.572	14.308	49.850	-629 -1089 2054 1.000 28.82
ANISOU				160	4020	3122	3807	-13 -966 - 90
ATOM ANISOU	1200		ARG ARG		0.649 1649	21.669	53.447	1.000 15.12
ATOM	1201		ARG		1.804	2863 21.556	1232 53.863	104 -66 125 1.000 17.09
ANISOU	1201	0	ARG		1291	3411	1791	-400 74 -812
ATOM	1202		PHE		-0.258	22.369	54.114	1.000 14.95
ANISOU ATOM	1202		PHE PHE		1512 -0.036	2506 22.949	1660 55.427	-253 -8 -146 1.000 13.27
ANISOU	1203	CA	PHE	161		1681	1760	-9 -249 - 4 1
ATOM	1204		PHE		-0.587	24.381	55.472	1.000 16.82
ANISOU ATOM	1204		PHE PHE		1594 -0.317	1947	2851	384 58 6 4
ANISOU			PHE		2464	25.109 2424	56.771 3684	1.000 22.56 -39 790 -1067
ATOM	1206	CD1	PHE		-1.175	25.010	57.849	1.000 26.03
ANISOU ATOM	1206 1207				3353	2919	3620	267 1106 - 702
ANISOU	1207	CD2	PHE		0.822 2353	25.901 3265	56.885 4011	1.000 25.34 -179 -161 - 738
ATOM	1208	CE1	PHE		-0.943	25.660	59.051	1.000 30.50
ANISOU					4784	3324	3481	-972 1456 - 620
ATOM ANISOU	1209	CE2			1.061 2546	26.553	58.080	1.000 26.10
ATOM	1210		PHE		0.199	3067 26.438	4302 59.164	-129 281 -1127 1.000 30.06
ANISOU	1210	CZ	PHE		3839	3197	4386	-152 774 -677
ATOM ANISOU	1211		PHE		-0.737		56.447	1.000 13.93
ATOM	1212		PHE PHE		1842 -1.916	1946 21.843	1503 56.270	-334 -277 - 240 1.000 18.26
ANISOU	1212	0	PHE		2000	3277	1662	-744 -399 4 7 5
ATOM	1213		ARG		-0.090	21.631	57.503	1.000 16.29
ANISOU ATOM	1213		ARG ARG		2063 -0.635	2516	1610	-937 -523 7 7
ANISOU			ARG		1772	20.719 2512	58.483 1650	1.000 15.62 -519 -266 7 6
ATOM	1215	С	ARG	162	-0.476	21.312	59.890	1.000 17.48
ANISOU ATOM	1215 1216		ARG ARG		1855	3131	1656	-603 -186 - 76
ANISOU			ARG		0.609 1928	21.734 3063	60.251 1557	1.000 17.23 -771 -42 -160
ATOM	1217	CB	ARG		0.081	19.374	58.458	1.000 21.99
ANISOU			ARG		3309	2318	2727	-272 -737 - 22
ATOM ANISOU	1218		ARG ARG		-0.573 3488	18.322 2375	59.348	1.000 26.07
ATOM	1219	CD	ARG		-0.231	16.896	4041 58.886	489 655 280 1.000 25.85
ANISOU			ARG	162	3106	2221	4495	418 -2 2 3 9
ATOM ANISOU	1220		ARG ARG		-0.943	15.916	59.698	1.000 28.83
WAT 200	1220	NE	DNA	102	4379	2437	4139	-181 332 -177





3.000	100	_				- 132 -			
ATOM	128	2 CA		18	1 6.396	7.168	60 676	1 000	0 16.12
ANISO ATOM	0 128	2 CA			1 2275	1958	1890	-171	<del>-3</del> 43 6 0 2
	128	3 CB	ALA	18	1 5.668	5.891	60.279		20.24
ANISO	0 128	3 CB		18:	1 2857	2158	2673	-648	
ATOM	158	4 C	ALA	18:	1 7.576	7.409	59.738		694 106 )15.43
ANISO			ALA		1 2223	1717	1925	-315	
ATOM	128	5 0	ALA		1 7.458	8.198	58.783	1 000	-369 4 3 2 ) 15 . 4 9
ANISO			ALA	18:	1 2268	1761	1858	-173	
ATOM	128	6 N	PRO	182	2 8.698	6.733	59.986		-296 4 3 4 16.03
ANISO			PRO	182	2 2517	1745	1829		8 5 3 1
ATOM	128	7 CD	PRO	182	8.983	5.802	61.101	1 000	19.61
ANISO	0 158	/ CD	PRO		2321	2908	2221		-306 1 2 4 0
ATOM	1288	B CA	PRO	182	9.865	6.907	59.076	1 000	14.78
ANISO	1200	S CA	PRO	182	2573	1336	1706	-101	-86 299
ANISO	1200	CB	PRO	182	10.914	5.948	59.649		16.20
ATOM			PRO		2570	1978	1607	170	-251 7 7
ANISO	1 1 2 0 0	CG	PRO	182		5.713	61.066		19.28
ATOM	129		PRO	182	2301	3071	1952	-199	-245 1001
ANISOU	1291		PRO	182	9.541	6.571	57.627	1 000	14.90
ATOM	1292		PRO	182	2230	1658	1772	-421	-262 3 4 0
ANISOU	1222		PRO	182	8.920	5.573	57.249		15.38
ATOM	1293		PRO	182		1587	1957	-467	-482 5 3 9
ANISOU	1223	74 (	HIS		9.969	7.460	56.730		12.28
ATOM	1294	C 2	HIS	183		1312	1617	-154	-284 1 5 6
ANISOU	1294	CA	HIS		9.733	7.354	55.300	1.000	11.90
ATOM	1295	CA	HIS	183		1495	1614	-254	-351 3 5
ANISOU	1295	CB	HIS	183	8.300	7.824	54.922		12.43
ATOM	1296	CC	HIS	183	1399	1368	1957	-128	
ANISOU	1296	CG	HIS HIS	183	8.168	9.314	55.089		11.36
ATOM	1297	CDS	TIC	103	1349	1369	1600	-367	-296 5 6
ANISOU	1297	CDS	HIC	103	8.259	10.374	54.249	1.000	12.03
ATOM	1298	ND1	HIC	103	1684 7.989	1296	1589	-43	157 - 10
ANISOU	1298	ND1	HIC	103	7.989 1901	9.858	56.339	1.000	13.27
$\mathtt{ATOM}$	1299	CE1	HTC		7.943	1439	1700	-65	267 193
ANISOU	1299	CE1	HTS	103	1939	11.187	56.244	1.000	12.43
ATOM	1300	NE2	PIR	183	8.101	1490	1296	77 -24	4 150
ANISOU	1300	NE2	HTS	183	1560	11.515	54.992	1.000	11.04
ATOM	1301	С	HIS	183	10.749	1437	1199	215	-232 4 8
ANISOU	1301	Ċ	HIS	183	1446	8.176	54.515	1.000	12.27
ATOM	1302	0	HIS	183	11.433	1639	1577	-303	-282 - 67
ANISOU	1302	0	HTS	183	1496	9.032 1915	55.064		12.94
ATOM	1303	N	TYR	184	10.849	7.907	1505	-558	-292 1 5
ANISOU	1303	N	TYR		1453	1027	53.215		10.61
ATOM	1304	CA	TYR		11.483	8.800	1552	-41	-380 1 1 0
ANISOU	1304	CA	TYR	184	1475	1104	52.256		11.36
ATOM	1305	CB	TYR		12.628	8.151	1738	-71	-264 1 7 8
ANISOU	1305	CВ	TYR	184	1631	1114	51.481 1734		11.79
MOTA	1306	CG	TYR		12.368	6.907		-62	-197 3 4
ANISOU	1306	CG	TYR	184	1680	921 16	50.677		11.29
ATOM	1307	CD1	ጥሃጽ	184	12.156	5.659			
ANISOU	1307	CD1	TYR	184	1663	927 18			11.76
ATOM	1308	CE1	ጥVR	184	11.911	4.526			
ANISOU	1308	CE1	TYR	184	1960	878 19	64   173	1.000	12.64
ATOM	1309	CD2	ጥሄጽ	184	12.333	6.949	49.279		182
ANISOU	1309	CD2	TYR	184	1252	1302	1674	1.000	11.13
ATOM	1310	CE2	TYR	184	12.102	5.834	48.502		-283 9 3
ANISOU	1310	CE2		184	1944	1422	1546	T.000	12.93
ATOM	1311	CZ	TYR	184	11.898	4.611		49 -38 1.000	4 / 5 1 2 1 4
ANISOU			TYR	184	1717	1304		30 -61	1 6 7
MOTA	1312	ОН	TYR	184	11.663	3.490		1.000	15 / 5 15 / 5
						•	-0.545	1.000	ı J . 4 D

- 133 -ANISOU 1312 OH TYR 184 2028 1471 2373 42 - 476 - 247 184 10.447 9.390 51.314 1.000 T.1.50 1313 C TYR ANISOU 1313 C TYR 184 1445 1215 1709 -187 -201 3 4 8 1314 0 TYR 8.797 51.089 -1.000 11.75 184 9.362 ANISOU 1314 O TYR 184 1305 1308 1853 -106 -171 4 2 7 185 10.784 10.557 50.743 1.000 10.79 1315 N ASP ANISOU 1315 N ASP 185 1581 1069 1449 -141 -132 1 1 8 1316 CA ASP 11.218 49.815 1.000 9.10 ATOM 185 9.861 ANISOU 1316 CA ASP 185 1089 1093 1277 -326 23 2 0 6 1317 CB ASP 185 9.934 12.743 49.886 1.000 10.13 ATOM ANISOU 1317 CB ASP 185 1427 1095 1327 -298 -178 1 7 7 1318 CG ASP 185 9.540 13.388 51.185 1.000 11.79 ATOM ANISOU 1318 CG ASP 185 1797 1350 1333 -250 -149 1 1 ATOM 1319 OD1 ASP 185 9.681 14.638 51.278 1.000 13.79 ANISOU 1319 OD1 ASP 185 2050 1316 1875 135 -52 - 26 1320 OD2 ASP 185 9.114 12.755 52.189 1.000 13.31 ANISOU 1320 OD2 ASP 1321 C ASP ANISOU 1321 C ASP 1322 0 MOTA ASP 185 1167 ASP ANISOU 1322 O -127 -35 -206LEU 186 9.038 LEU 186 1211 1323 N ATOM ANISOU 1323 N ANISOU 1323 N LEU 186 1211 1186 1437 -272 -177 ATOM 1324 CA LEU 186 9.124 10.312 46.161 1.000 10.60
ANISOU 1324 CA LEU 186 1641 986 1401 -239 -52 - 44
ATOM 1325 CB LEU 186 8.030 9.295 45.798 1.000 11.32 1186 1437 -272 -177 - 58 ANISOU 1325 CB LEU 186 1652 929 1721 -111 17 -479 ATOM 1326 CG LEU 186 7.989 7.977 46.602 1.000 12.60 ANISOU 1326 CG LEU 186 1408 1039 2340 -263 -200 --263 -200 - 166 1327 CD1 LEU 186 6.896 7.064 46.028 1.000 16.64 ANISOU 1327 CD1 LEU 186 1900 1373 3049 -634 -398 - 135 1328 CD2 LEU 186 9.356 7.332 46.629 1.000 13.84 MOTA ANISOU 1328 CD2 LEU 186 1438 1245 2575 -155 443 283 1329 C LEU 186 9.024 11.521 45.223 1.000 10.90 MOTA ANISOU 1329 C LEU 186 1327 1603 1211 -3 -451 164 1330 O MOTA LEU 186 8.768 11.406 44.031 1.000 13.60 ANISOU 1330 O LEU 186 2067 1608 1494 -211 -321 1 0 3 1331 N SER 187 9.264 12.705 45.734 1.000 10.71 MOTA ANISOU 1331 N 1331 N SER 187 1546 1129 1393 -76 -282 3 1332 CA SER 187 9.401 13.943 44.998 1.000 10.49 -282 3 1 8 ATOM 1333 CB SER 187 1427 1191 1370 195 -107 4
ANISOU 1333 CB SER 187 1105 1048 1857 200 10.56
ANISOU 1334 OG SEP 187 127 -107 4 8 8 1333 CB SER 187 1105 1048 1857 298 161 5 1334 OG SER 187 10.430 14.918 46.726 1.000 13.01 161 532 ANISOU 1334 OG SER 187 1343 1432 2169 -132 -295 2 ATOM 1335 C SER 187 10.774 14.062 44.336 1.000 10.47 -132 -295 2 0 1 SER 187 10.774 14.062 44.336 1.000 10.47

SER 187 1447 862 1669 135 -3 145

SER 187 11.684 13.246 44.513 1.000 10.54

SER 187 1577 799 1629 183 -91 - 77

MET 188 10.962 15.095 43.502 1.000 9.78

MET 188 1419 978 1318 147 44 7 4

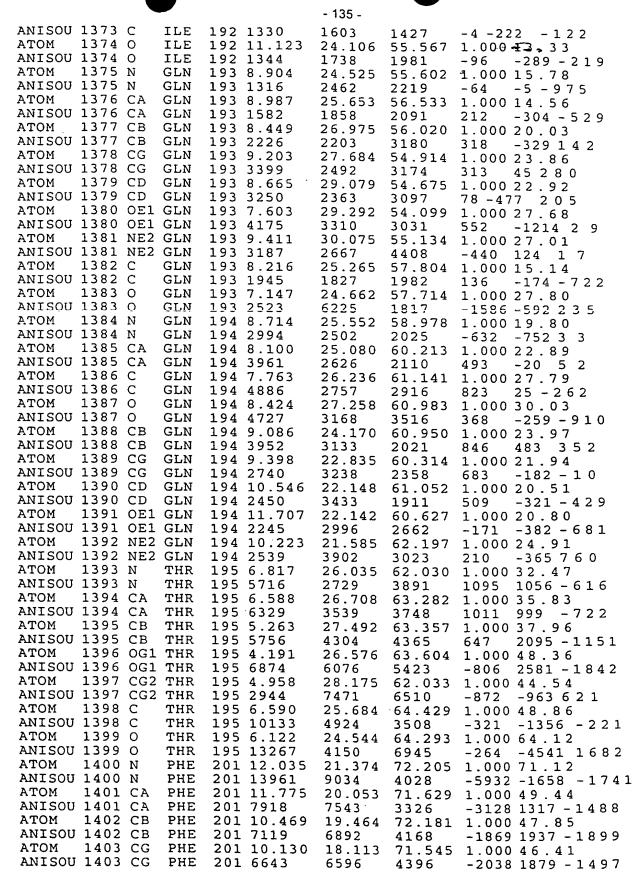
MET 188 12.267 15.584 43.065 1.000 9.94

MET 188 1394 942 1441 182 58 3 7

MET 188 1523 840 1774 98 48 2 2 7

MET 188 13.385 17 258 41 470 1 000 11 40 ANISOU 1335 C MOTA 1336 0 ANISOU 1336 O 1337 N MOTA ANISOU 1337 N 1338 CA MOTA ANISOU 1338 CA 1339 CB MOTA ANISOU 1339 CB 1340 CG 188 13.385 17.258 41.470 1.000 11.40 ATOM MET ANISOU 1340 CG MET 188 1403 1172 1756 46 -51 214 MOTA 1341 SD MET 188 14.687 16.134 40.891 1.000 12.71 ANISOU 1341 SD 188 1619 MET 1272 1940 139 137 198 188 16.061 17.267 40.790 1.000 13.86 1342 CE ATOM MET ANISOU 1342 CE MET 188 1862 1399 2003 -2911 - 90

						- 134 -		
ATOM	1343	С	MET	188	12.946	16.217	44 201	1 000 10 10
ANISOU	1343	С	MET		1325	1586		1.000 12.13
ATOM	1344	0	MET		13.971	15.727	1698	16918 - 285
ANISOU	1344	0	MET	188		1553	44.804	1.000 11.52
ATOM	1345		VAL		12.362	17.290	1535	144 132 8 7
ANISOU			VAL		1290	17.290	44.838	1.000 10.00
ATOM	1346		VAL		12.745	17.894	1292	53 -175 6
ANISOU	1346	CA	VAL		1209		46.099	1.000 9.70
ATOM	1347		VAL		13.618	1057 19.154	1420	-212 -45 -19
ANISOU	1347	СB	VAL		1288	19.154	45.979	1.000 9 . 9 7
ATOM	1348		VAT.		14.953	18.837	1398	-238 129 189
ANISOU	1348	CG1	VAL	189	1334	1410	45.266	1.000 13.45
ATOM	1349	CG2	VAT.		12.899	20.289	2368	-236 390 143
ANISOU	1349	CG2	VAL		1715	1242	45.264 1693	1.000 12.24
ATOM	1350	С	VAL		11.469	18.245	46.871	-25 150 295
ANISOU			VAL		1089	1600	1149	1.000 10.10
ATOM	1351	0	VAL		10.405	18.399	46.250	-456 -156 - 73
ANISOU			VAL		1153	1249	1217	1.000 9.53 -222 -190 8
ATOM	1352	N	THR		11.609	18.327	48.187	
ANISOU	1352	N	THR		1273	894 11		1.000 8.66 -202 127
ATOM	1353	CA	THR		10.565	18.771	49.091	-202 127 1.0009.64
ANISOU		CA	THR		1350	1167	1147	
MOTA	1354	CB	THR	190	10.194	17.699	50.132	-11 -228 - 9 9 1.000 10.69
ANISOU		CB	THR	190	1231	1196	1635	
ATOM	1355	OG1	THR	190	9.662	16.586	49.501	-300 121 - 54 1.000 12.45
ANISOU	1355	OG1	THR	190	1333	1341	2055	
ATOM	1356	CG2	THR		9.038	18.131	51.019	-140 -258 - 48 1.000 13.59
ANISOU	1356	CG2	THR	190	1121	2222	1821	
ATOM	1357	С	THR	190	11.058	19.976	49.891	-272 151 -195 1.000 9.23
ANISOU	1357	С	THR		1257	1096	1152	-102 -336 - 49
ATOM	1358		THR		12.149	19.867	50.447	1.000 10.54
ANISOU		0	THR	190	1322	1292	1390	-5 -359 -122
ATOM	1359	N	LEU	191	10.313	21.064	49.978	1.000 10.23
ANISOU			LEU	191	1319	1167	1401	-71 -177 - 1 3 3
ATOM	1360	CA	LEU	191	10.691	22.241	50.770	1.000 10.19
ANISOU	1360	CA	LEU		1259	1176	1438	0 -294 -142
ATOM	1361		LEU	191	10.604	23.511	49.910	1.000 11.52
ANISOU		CB	LEU		1203	1185	1990	-118 -601 3 2
ATOM	1362	CG	LEU	191	11.897	23.898	49.167	1.000 13.23
ANISOU		CG	LEU		1898	1710	1419	-391 -358 9 7
ATOM	1363	CD1	LEU		12.333	22.794	48.218	1.000 15.25
ANISOU					1685	2018	2091	-476 -214 - 305
ATOM	1364	CD2	LEU		11.717	25.231	48.448	1.000 17.46
ANISOU	1364	CD2			2310	2044	2281	-14 17 6 0 4
ATOM	1365		LEU		9.798	22.328	52.006	1.000 11.93
ANISOU		C	LEU		1275	1677	1579	56 - 190 - 372
ATOM		0	LEU		8.560	22.262	51.868	1.000 13.49
ANISOU		0	LEU		1276	2173	1676	1 -192 -601
ATOM		N	ILE	192	10.394	22.483	53.190	1.000 11.06
ANISOU ATOM		N	ILE		1115	1603	1487	-111 -92 -108
	1368	CA	ILE	192	9.671	22.539	54.443	1.000 11.13
ANISOU ATOM			ILE	192	1071	1638	1521	11 -173 - 149
ANISOU	1369	CR	ILE	192	9.927	21.304	55.330	1.000 12.94
ATOM			ILE		2099	1586	1232	-65 -9 -233
	1370	CGZ	ILE	192	9.221	21.428	56.673	1.000 16.06
ANISOU ATOM	1371 1371	002	TLE	192	2479	1983	1641	-206 426 -215
	1371	CGI	TLE	192	9.512	20.028	54.590	1.000 15.51
ANISOU ATOM	1377	CGT	TLE		2633	1658	1601	-400 -48 -175
	1372	CDI	TLE		9.845	18.765	55.339	1.000 25.71
ANISOU ATOM	1372	CDI			5869	1608	2290	-175 -1566 - 301
ATOM	1373	C	ILE	192	9.966	23.809	55.253	1.000 11.47

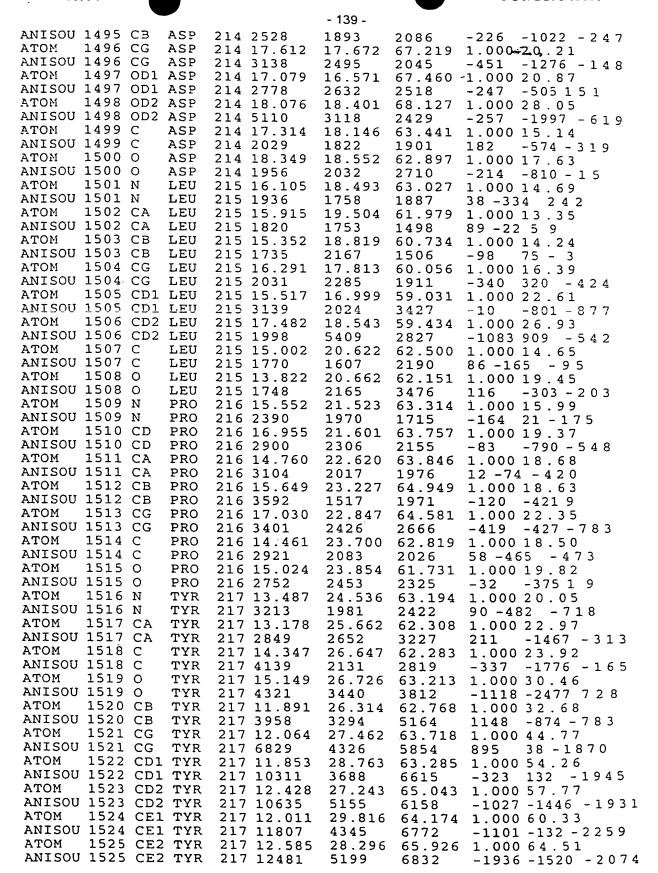


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ATOM	1404	CD1	PHE	201	10.738	16.954	71 001	1 000 50 00
ANISOU	1404	CD1	PHE		7982	6634	71.991 4393	
ATOM	1405	CD2	PHE		9.220	18.001	70.513	-2326-1992 - 991 1.000 42.63
ANISOU	1405	CD2	PHE		5458	6427	4313	-1097 2449 - 2268
ATOM	1406	CE1	PHE	201	10.434	15.739	71.417	1.000 49.95
ANISOU	1406	CE1	PHE	201	8275	6464	4240	-2047 227 -716
ATOM	1407	CE2	PHE		8.901	16.783	69.934	1.000 41.38
ANISOU	1407	CE2			6016	5946	3762	-578 2006 - 1844
ATOM ANISOU	1408	CZ	PHE		9.515	15.636	70.392	1.000 44.74
ATOM	1408		PHE		7075	6261	3663	-1063 1020 - 975
ANISOU			PHE PHE	201	11.722	20.110	70.107	1.000 42.42
ATOM	1410		PHE		6324 11.007	6442	3351	-1964 717 -1441
ANISOU			PHE		9668	20.941 4400	69.536	1.000 47.79
ATOM	1411	N	VAL		12.477	19.232	4090 69.449	-762 691 -2416
ANISOU			VAL	202	4525	5852	2558	1.000 34.04 -1948 7 -425
ATOM	1412	CA	VAL		12.535	19.245	67,993	1.000 25.09
ANISOU			VAL		3221	3752	2558	-1041 -182 9 9
ATOM	1413		VAL	202	13.988	19.286	67.489	1.000 22.88
ANISOU ATOM			VAL		2832	3430	2432	-577 -691 -198
ANISOU	1414	CGI	VAL	202	14.053	19.387	65.965	1.000 26.02
ATOM	1415	CGI	VAL		3821	3594	2470	-958 35 -277
ANISOU	1415	CG2	VAL VAL		14.771 3043	20.443	68.078	1.000 24.69
ATOM	1416	C	VAL		11.798	3473	2867	-786 -410 - 320
ANISOU	1416	č	VAL	202	3027	18.035 2810	67.421 2023	1.000 20.69
ATOM	1417	0	VAL	202	12.288	16.914	67.581	-648 58 6 1 5 1.000 26.08
ANISOU			VAL	202	3294	3219	3396	-136 452 884
ATOM	1418	N	SER		10.662	18.234	66.766	1.000 20.21
ANISOU			SER		3100	2794	1787	-414 25 -152
ATOM	1419	CA	SER		9.820	17.192	66.218	1.000 20.37
ANISOU ATOM	1419		SER		3149	2709	1884	-355 129 -256
ANISOU	1420	CB	SER	203	8.437	17.779	65.896	1.000 24.72
ATOM	1421		SER SER		2726	4106	2558	-178 369 -1015
ANISOU	1421	06	SER		7.841 3328	18.239	67.097	1.000 31.80
ATOM	1422		SER		10.367	5782 16.524	2974	-457 1175 -1104
ANISOU	1422	Ċ	SER		2580	2647	64.958 2040	1.000 19.13
ATOM	1423	0	SER		10.279	15.302	64.832	-339 170 -244 1.000 17.01
ANISOU		0	SER		2311	2625	1527	-414 206 - 18
ATOM	1424		LEU	204	10.902	17.259	63.998	1.000 16.16
ANISOU			LEU	204	2142	1976		71 77 - 292
ATOM	1425	CA	LEU		11.403	16.679	62.740	1.000 14.07
ANISOU ATOM	1425		LEU		1670	1626	2049	-22 -24 -283
ANISOU	1426	CB	LEU		11.269	17.704	61.618	1.000 13.80
ATOM		CG	LEU LEU		1549	1763	1931	-249 -340 - 277
ANISOU		CG	LEU		11.647 1726	17.272	60.212	1.000 14.13
ATOM		CD1			10.770	1722 16.134	1919	-253 -482 -412
ANISOU		CD1	LEU		2579	2895	59.680 1654	1.000 18.76
ATOM	1429	CD2	LEU		11.609	18.478	59.255	-1297 -927 - 106 1.000 16.20
ANISOU	1429	CD2	LEU	204	1987	2095	2074	65 75 -123
MOTA	1430	С	LEU		12.832	16.140	62.885	1.000 14.81
ANISOU			LEU	204	1734	1748	2144	9 -199 -250
ATOM		0	LEU		13.699	16.853	63.397	1.000 15.52
ANISOU ATOM		0	LEU		1833	1789	2274	-59 -435 - 42
ANISOU		N	GLN		13.065	14.900	62.469	1.000 14.42
ATOM	1433	N C A	GLN GLN		1847	1804	1827	189 -120 - 153
ANISOU	1433	CA	GLN		14.288 1777	14.143	62.574	1.000 12.76
ATOM	1434		GLN		14.622	1655 13.434	1419	43 - 347 - 113
						T1.424	61.260	1.000 11.12

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						- 137 -		
NOSIMA	1434	С	GLN	205	1412	1474	1338	49 -468 - 21
MOTA		0	GLN	205	13.707	12.927	60.606	1.000- <del>1</del> 3, 97
ANISOU		0	GLN	205	1622	2235	1449	-293 -449 - 147
MOTA	1436	CB	GLN	205	14.164	13.062		1.000 15.57
ANISOU	1436	CB	GLN		2421	1925	1568	341 151 8 3
ATOM	1437	CG	GLN	205	13.863	13.635	65.032	1.000 18.58
ANISOU	1437	CG	GLN	205	3321	2286	1451	689 -129 8 2
MOTA	1438	CD	GLN	205	15.086	14.243	65.680	1.000 24.33
ANISOU	1438	CD	GLN	205	3687	3465	2091	520 -499 - 570
ATOM	1439	OE1	GLN	205	16.206	13.717	65.549	1.000 29.12
ANISOU		OE1		205	3350	3464	4251	14 -270 -1800
MOTA	1440			205	14.840	15.356	66.378	1.000 23.01
NOSINA					3055	2465	3225	335 -592 - 140
MOTA		N	ALA		15.893	13.401	60.893	1.000 12.63
ANISOU			ALA		1523	1770	1506	-251 -234 - 6
ATOM		CA	ALA		16.335	12.649	59.731	1.000 13.77
ANISOU		CA	ALA		1392	2099	1742	-522 -72 -295
ATOM	1443	CB	ALA		16.693	13.519	58.528	1.000 16.34
ANISOU			ALA		2034	2494	1682	-603 123 -277
ATOM	1444		ALA		17.567	11.813	60.046	1.000 15.92
ANISOU		C	ALA		1489	2331	2230	-290 179 -341
ATOM		0	ALA		18.368	12.182	60.908	1.000 15.86
ANISOU		0	ALA		1877	1772	2377	150 -356 3 0
ATOM		N	GLU		17.707	10.712	59.305	1.000 16.98
ANISOU ATOM	1447	N	GLU		1981	2086	2383	-335 348 -186
ANISOU		CA	GLU		18.938	9.942	59.364	1.000 20.58
ATOM	1448	C	GLU GLU		2198	1938	3684	-164 490 -10
ANISOU		C	GLU		20.082 1828	10.688	58.681	1.000 18.75
ATOM		ō	GLU		19.948	2037 10.953	3260	272 185 5 5 8
ANISOU		Ö	GLU	207		2145	57.503	1.000 18.23
ATOM		СВ	GLU	207	18.665	8.612	3034 58.676	528 - 45 1.000 25.81
ANISOU			GLU		3289	1794	4724	-19 83 - 135
ATOM	1451	ĊĞ	GLU		19.879	7.737	58.429	1.000 30 . 08
ANISOU		CG	GLU	207		2221	5105	907 -948 - 546
ATOM	1452	CD	GLU	-	19.429	6.356	57.959	1.000 29.93
UOZINA		CD	GLU		5549	2024	3798	1179 -2099 -123
MOTA	1453	OE1			19.491	5.471	58.839	1.000 35.14
ANISOU	1453	OE1			5782	2692	4879	938 -931 8 8 5
MOTA	1454			207		6.251	56.762	1.000 38.62
ANISOU	1454	OE2	GLU	207		5608	4109	135 -2494 - 366
MOTA	1455	N	VAL	208	21.146	10.997	59.414	1.000 16.97
ANISOU			VAL		1926	1974	2549	120 337 807
ATOM	1456	CA	VAL		22.376	11.593	58.902	1.000 17.77
ANISOU			VAL		1894	2109	2748	93 500 4 1 1
ATOM	1457		VAL		22.455	13.111	59.155	1.000 16.89
ANISOU			VAL		2774	2148	1494	-372 -149 5 6 9
ATOM	1458				23.652	13.688	58.409	1.000 20.76
ANISOU					3214	2150	2526	-423 647 148
MOTA	1459				21.172	13.815	58.720	1.000 16.36
ANISOU					3146	1640	1431	25 98 3 5 3
ATOM	1460		VAL		23.585	10.877	59.507	1.000 20.29
ANISOU			VAL		1936	2555	3217	11 -58 1 3 2
ATOM	1461		VAL		23.726	10.829	60.741	1.000 20.74
ANISOU			VAL		2436	2256	3187	460 206 544
ATOM	1462		GLY	209	24.457	10.295	58.672	1.000 18.94
ANISOU ATOM	1462		GLY		1764	2445	2989	211 -494 1 5
ANISOU			GLY		25.558	9.508	59.194	1.000 24.01
ATOM	1463		$\mathtt{GLY}$		2171	3040	3910	549 -396 7 0 9
ANISOU			GLY		25.123 2874	8.364	60.082	1.000 25.00
*7117300	7404	_	GWI	209	2014	3156	3470	1406 772 649

ATOM 1465 O	O		- 138 -		
ANISOU 1465 O		25.850	7.934	60.991	1.000 35.98
ATOM 1466 N		4448	3946	5279	1425-426 1769
ANISOU 1466 N		23.951	7.786	59.869	1.000 25.89
ATOM 1467 CA		3802 23.477	2756	3278	523 899 749
ANISOU 1467 CA		23.4// 4479	6.678	60.671	1.000 26.43
ATOM 1468 C		22.885	2136 7.025	3427	1228 742 912
ANISOU 1468 C		5472	2099	62.016 3237	1.000 28.45
ATOM 1469 O		22.634	6.098		831 1029 1175
ANISOU 1469 O	GLY 210	7322	2719	62.789 5256	1.000 40.26
ATOM 1470 N		22.651	8.281	62.338	1881 2759 2360
ANISOU 1470 N		4671	2359	2763	1.000 25.78 1370 724 1197
ATOM 1471 CA		22.048	8.671	63.613	1370 724 1197 1.000 23.74
ANISOU 1471 CA	ALA 211	2966	3156	2896	727 339 663
ATOM 1472 CB		23.093	9.333	64.496	1.000 29.57
ANISOU 1472 CB		2957	4372	3906	834 -96 6 9
ATOM 1473 C		20.900	9.626	63.360	1.000 21.19
ANISOU 1473 C ATOM 1474 O		3090	2611	2350	484 178 741
ANISOU 1474 O		20.936	10.381	62.399	1.000 23.91
ATOM 1474 O		3771	2659	2653	-30 -66 930
ANISOU 1475 N		19.889	9.629	64.204	1.000 19.88
ATOM 1476 CA		2603 18.814	2577	2375	398 -128 3 7 4
ANISOU 1476 CA	PHE 212	2581	10.613 2257	64.130	1.000 19.13
ATOM 1477 C		19.320	12.006	2432	284 -565 3 1 7
ANISOU 1477 C		3004	2480	64.489 2115	1.000 20.00 133 -640 6 8
ATOM 1478 O		19.893	12.230	65.569	133 -640 6 8 1.000 21.10
ANISOU 1478 O	PHE 212	2497	3558	1964	-391 -406 2 2 2
ATOM 1479 CB	PHE 212	17.688	10.290	65.096	1.000 21.37
ANISOU 1479 CB		2553	2616	2952	293 -197 - 184
ATOM 1480 CG ANISOU 1480 CG		17.010	8.950	64.912	1.000 23.45
ATOM 1481 CD1	PHE 212	2161	3496	3253	-376 -282 - 558
ANISOU 1481 CD1		16.369 2545	8.377	65.990	1.000 23.33
ATOM 1482 CD2		2345 17.029	3115	3206	-382 -350 - 508
ANISOU 1482 CD2		2554	8.302 3962	63.687	1.000 25.83
ATOM 1483 CE1		15.730	7.149	3299 65.872	-622 -217 - 787
ANISOU 1483 CE1		3784	3544	3362	1.000 28.13 -1119 96 - 973
ATOM 1484 CE2	PHE 212		7.072	63.569	1.000 23.04
ANISOU 1484 CE2	PHE 212	2504	2960	3289	382 -232 - 558
ATOM 1485 CZ	PHE 212	15.781	6.486	64.651	1.000 27.88
ANISOU 1485 CZ		3658	3977	2957	-1072 -501 - 760
ATOM 1486 N	THR 213	19.076	12.936	63.578	1.000 18.30
ANISOU 1486 N ATOM 1487 CA		2690	2083	2181	149 -583 - 93
ANISOU 1487 CA	THR 213 THR 213	19.566	14.310	63.681	1.000 17.99
ATOM 1488 CB		1976	2139	2721	230 -686 - 287
ANISOU 1488 CB		20.515 1798	14.586	62.498	1.000 20.43
ATOM 1489 OG1		21.638	2280 13.695	3683	140 -119 - 423
ANISOU 1489 OG1		2571	3378	62.629 3676	1.000 25.33
ATOM 1490 CG2	THR 213	21.087	15.985	62.485	925 71 5 2 8 1.000 21.11
ANISOU 1490 CG2		1935		3420	-310 -289 - 747
ATOM 1491 C	THR 213	18.391	15.277	63.641	1.000 15.53
ANISOU 1491 C		1732	2135	2032	111 -557 - 167
ATOM 1492 O		17.533	15.195	62.761	1.000 16.11
ANISOU 1492 O ATOM 1493 N		1742	2197	2180	-327 -669 5 6
ANISOU 1493 N		18.362	16.199	64.590	1.000 15.60
ATOM 1494 CA		2025 17.380	2046	1857	64 -405 2
ANISOU 1494 CA		2130	17.256 1722	64.672 2072	1.000 15.59
ATOM 1495 CB		17.744	18.200		2 -1010 - 242 1.000 17.13
	_ <b>-</b>			JJ. 0 Z Z	1.000 17.13



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ATOM	1526	CZ	TYR	217	12.378	29.586	65.481	1.000 64.11
JOSINA MOTA			TYR		12047	5183	7129	-1460 < 817 - 2160
ATOM	1527	OH	TYR		12.536	30.639	66.358	1.000 63.69
ATOM	1528		TYR		11840	5206	7153	-1832 -1191 -206
ANISOU	1526 1526	V1 6	ARG	218		27.374	61.188	1.000 24.08
ATOM	1529		ARG		4482	1611	3055	507 -1471 - 145
ANISOU	1 1529		ARG ARG		15.335	28.465	60.948	1.000 30 . 71
ATOM	1530		ARG		5932 16.326	2490	3245	-504 -1565 382
ANISOU	1530	CB	ARG	210	5969	28.135	59.840	1.000 35.08
ATOM	1531	CG	ARG		17.401	2797 27.114	4562	-1397 -779 - 348
ANISOU	1531	CG	ARG	218	6009	3087	60.073	1.000 35.77
ATOM	1532		ARG	218	18.658	27.775	4497 60.626	-1107 -733 - 773
ANISOU			ARG	218	5680	3264	4152	1.000 34.46
ATOM	1533	NΞ	ARG		19.223	28.746	59.709	-1242 -244 - 619 1.000 29.51
ANISOU			ARG	218	4707	2579	3926	78 81 -629
ATOM	1534	CZ	ARG	218	20.218	28.620	58.830	1.000 33.18
ANISOU ATOM	1534	CZ	ARG		5269	3166	4170	60 452 -1075
ANISOU	1535	NHI	ARG	218	20.839	27.452	58.709	1.000 27.44
ATOM	1536	MRO	ARG	218	4202	2881	3341	-503 -373 -1585
ANISOU	1536	NHO	ARG	218	20.583	29.675	58.077	1.000 22.96
ATOM	1537	C	ARG		2327 14.513	3579	2817	233 -1117 -872
ANISOU	1537	Č	ARG	210	7353	29.655	60.464	1.000 31.05
ATOM	1538	0	ARG		14.114	1949 29.533	2496	-448 -1823 197
ANISOU			ARG	218	9873	2241	59.295 3235	1.000 40.40
ATOM	1539	N	PRO		14.246	30.747	61.157	531 -3168 - 627
ANISOU			PRO	219	6290	2559	2555	1.000 30.01 -499 -1839 -284
ATOM	1540	CD	PRO	219	14.597	31.043	62.543	-499 -1839 -284 1.000 36.79
ANISOU			PRO		8147	2878	2954	-1848 -2548 - 374
ATOM ANISOU	1541	CA	PRO	219	13.464	31.841	60.549	1.000 26.34
ANISOU	1541		PRO		4421	2564	3025	-573 -988 - 340
ANISOU	1542	CB	PRO	219	13.523	32.993	61.563	1.000 32.44
ATOM	1543		PRO PRO		5361	2891	4073	-691 -417 - 989
ANISOU	1543	CG	PRO		13.947 7916	32.372	62.825	1.000 38.75
ATOM	1544	C	PRO		14.005	3462	3344	-1981 -958 -1235
ANISOU	1544	Č	PRO	219	3472	32.329 2066	59.220	1.000 23.64
ATOM	1545	Ō	PRO		13.300	32.950	3443	-161 -1028 1 0 9
ANISOU		0	PRO	219	4358	2934	58.412 4339	1.000 30.61
ATOM	1546	N	ASP		15.269	32.087	58.906	-347 -1712 8 7 6 1.000 25.98
ANISOU			ASP		3611	1756		-389 -644 <b>-</b> 815
MOTA	1547	CA	ASP		15.847	32.660	57.705	1.000 27.96
ANISOU ATOM	1547	CA	ASP	220	3951	1603	5071	-364 30 -824
ANISOU	1548	CB	ASP	220	17.212	33.238	58.155	1.000 29.61
ATOM	1548	CB	ASP		3549	3142	4558	-176 -326 1 7 6
ANISOU	1549	CC	ASP ASP		18.091	32.158	58.780	1.000 32.09
ATOM	1550	001	ASP		3706	3527	4961	625 978 615
ANISOU	1550	OD1	ASP	220	17.697 3013	31.434	59.719	1.000 26.12
ATOM	1551	OD2	ASP		19.241	3522	3390	-158 -289 - 97
ANISOU	1551	OD2	ASP	220	3714	32.088 3756	58.281	1.000 29.09
ATOM	1552	С	ASP	220	16.037	31.726	3581	304 677 - 712
ANISOU	1552	C	ASP	220	2508	1291	56.525 5800	1.000 25.26
ATOM	1553	0	ASP		16.641	32.095	55.515	354 1110 - 822
ANISOU	1553	Ο.	ASP	220	4088	1665	4994	1.000 28.28 -855 298 -434
ATOM	1554	N	ALA	221	15.500	30.510	56.631	1.000 21.58
ANISOU			ALA	221	2748	1770	3681	-288 178 -651
ATOM	1555	CA	ALA	221	15.840	29.484	55.658	1.000 19.81
ANISOU ATOM			ALA		2986	1452	3090	-342 -224 - 315
OF1	1556	CB	ALA	221	17.130	28.800	56.109	1.000 19.51

- 141 -ANISOU 1556 CB ALA 221 2267 1497 3647 -648 45 - 746 1557 C ALA 221 14.718 28.469 55.489 1.000-17.71 1557 C ALA 221 2304 1912 2512 -251 -75 -309 ANISOU 1557 C 1558 O ATOM ALA 221 13.866 28.356 56.380-1.000 20.97 ANISOU 1558 O ALA 221 3596 2029 2344 -503 406 -284

ANISOU 1584 CG PHE 225 964 1369 1991 -251 -333 181
ATOM 1585 CD1 PHE 225 14.685 15.653 54.291 1.000 15.28
ANISOU 1585 CD1 PHE 225 1771 1777 2256 -98 -853 2 9
ATOM 1586 CD2 PHE 225 12.532 16.576 54.254 1.000 17.91

ANISOU 1586 CD2 PHE 225 1904 2748 2153 341 106 0

2256 -98 -853 2 9 8

						- 142 -		
ATOM	1587	CE1	PHE		14.619	15.535	55 661	1.000 17.46
ANISOU	J 1587	CE1	PHE	225	2449	1862	2321	
ATOM	1588	CE2	PHE	225	12.447		55 612	-249. <u>-7</u> 95 6 6 6 1.000 19.35
ANISOU	7 1588	CE2		225	2563	2678	2111	1.000 19.35
ATOM	1589	CZ	PHE		13.499	15.945	56.341	
ANISOU	1589	CZ	PHE	225	2952	1641	2324	
ATOM	1590	С	PHE		14.907	16.774	40 007	-501 -470 3 6
ANISOU			PHE	225	1480	1285		1.000 12.03
ATOM	1591	0	PHE	225	14.019	17.160		
ANISOU			PHE	225	1473		49.163	1.000 12.77
ATOM	1592	N	CYS		15.940			341 -118 3 8
ANISOU			CYS	226	954 140		96 -2	1.000 9 . 6 2
ATOM	1593	CA	CYS	226	15.917	15 400	10 107	04 -407 2 9 1.000 10.80
ANISOU			CYS	226	1432	1204	1468	1.000 10.80
ATOM	1594	CB	CYS		17.337	15.029		
ANISOU			CYS	226	1539	1362		1.000 12.02
ATOM	1595	SG	CYS	226	18.426			-357 16 -125 1.000 13.74
ANISOU			CYS	226	1627	1400	2192	
ATOM	1596	С	CYS	226	14.998	14.178	48.256	
ANISOU	1596	С	CYS	226	1190	1061	1495	_ <del>_</del>
ATOM	1597	0	CYS		15.015	13.431		-20 -293 - 16 1.000 11.17
ANISOU			CYS	226	1181	1280	1781	
ATOM	1598	N	$\mathtt{GLY}$		14.217	13.963	47.205	
ANISOU			${ t GLY}$	227	1428	1010		-258 -271 - 35
ATOM	1599	CA	${ t GLY}$	227	13.370		47 053	1.000 9 . 7 3
ANISOU			${ t GLY}$	227	1231	860 16	04 -15	78 -74 - 3 7
ATOM	1600	С	$\mathtt{GLY}$	227	13.908	11.769	46 074	1.000 9 . 4 8
ANISOU			GLY	227	1438	717 14	45 16	-35 169
ATOM	1601	0	$\mathtt{GLY}$	227	14.935	11.961		1.000 9 . 8 6
ANISOU			$\mathtt{GLY}$	227	1321	1137	1290	-104 -179 7 8
ATOM	1602	N	ALA	228	13.217	10.631	45.971	1.000 9.17
ANISOU			ALA		1279	729 14	77 109	-135 5 8
ATOM	1603	CA	ALA	228	13.650	9.529		1.000 9 . 41
ANISOU			ALA		1315	887 13	71 9	-74 - 5 2
ATOM	1604	CB	ALA	228	12.727	8.296	45.256	1.000 10.50
ANISOU			ALA	228	2011	824 11	55 -14	3 124 1 0 1
ATOM	1605	C	ALA	228	13.712	9.918	43.637	1.000 9.25
ANISOU	1605	C	ALA		1343	666 150	07 -10	08 90 1 3 9
ATOM	1606	0	ALA	228	14.493	9.305		1.000 9 . 4 8
ANISOU ATOM			ALA	228	1171	1026	1405	-88 -50 9 0
	1607	N	ILE	229	12.970	10.907	43.143	1.000 10.30
ANISOU	1607		ILE	229	1402	1004	1509	18 25 177
ATOM ANISOU	1008	CA	ILE	229	13.074	11.311	41.727	1.000 10.87
ATOM			ILE	229	1197	1446	1487	-2 -159 251
ANISOU	1609	CB	ILE	229	11.802	12.078	41.295	1.000 11.52
ATOM	1610		ILE	229		1473	1647	34 - 57 3 6 2
ANISOU	1610		ILE	229		12.852	39.999	1.000 11.30
ATOM	1611	CGZ	ILE	229		1211	1426	83 - 189 156
ANISOU	1611			229		11.131	41.237	1.000 14.39
ATOM	1612	CGI	ILE	229		2034	2402	-40 210 311
ANISOU	1612			229	10.676	10.093	40.138	1.000 19.20
ATOM			ILE	229		1723	3489	-610 93 - 138
ANISOU	1613	C	ILE	229		12.034	41.477	1.000 10.38
ATOM	1614		ILE	229		1405	1247	-62 -169 3 2 2
ANISOU	1614	0	ILE	229		11.947	40.369	1.000 11.66
ATOM		N	ILE	229		1257	1368	-13 145 328
ANISOU	1615		ALA	230		12.692	42.490	1.000 10.66
ATOM	1616		ALA	230		1274	1300	-104 -151 3 5 6
ANISOU	1616	CA	ALA	∠3U		13.259	42.338	1.000 11.21
ATOM	1617	CR	ALA	230		975 18:		
	-01/	CD	ALA	2 <b>3</b> U	16.681	14.148	43.509	1.000 10.58

- 143 -ANISOU 1617 CB ALA 230 1350 1295 62 - 106 1 2 6 1375 1618 C ALA 230 17.336 12.136 42.132 1.000 1-1,28 1610 ANISOU 1618 C ALA 230 1640 1037 1 55 2 4 2 1619 0 ALA 230 18.220 12.185 41.273 1.000 11.29 1539 -189 -40 288 ANISOU 1619 O ALA 230 1510 1240 1620 N THR 231 17.173 11.097 42.946 1.000 10.55 ATOM 1620 N THR 231 1328 894 1787 -262 -70 2 1 4 1621 CA THR 231 18.064 9.939 42.819 1.000 11.98 ANISOU 1620 N ATOM 
 231
 18.064
 9.939
 42.819
 1.000 11.98

 231
 1929
 1018
 1605
 0 -164
 159

 231
 17.717
 8.865
 43.878
 1.000 10.76

 231
 1381
 1070
 1636
 -86
 -453 2 4 6

 231
 17.658
 9.437
 45.198
 1.000 11.82

 231
 1615
 1236
 1641
 35 -115
 2 7 7

 231
 18.765
 7.752
 43.880
 1.000 12.57

 231
 1621
 1314
 1840
 160 -89
 3 5 1

 231
 17.958
 9.352
 41.415
 1.000 12.52

 231
 1632
 1500
 1624
 -145
 42.1
 ANISOU 1621 CA THR ATOM 1622 CB THR ANISOU 1622 CB THR ANISOU 1622 CB THR ATOM 1623 OG1 THR ANISOU 1623 OG1 THR 1624 CG2 THR MOTA ANISOU 1624 CG2 THR 1625 C MOTA THR ANISOU 1625 C 231 1632 1500 THR 1624 -145 42 1 1 231 18.939 9.050 40.732 1.000 12.15 MOTA 1626 O THR ANISOU 1626 O THR 231 1636 1233 1747 -17 86 2 2 4 1627 N 232 16.717 9.154 40.959 1.000 11.14 MOTA LEU ANISOU 1627 N LEU 232 1608 1005 1620 90 - 68 1 4 1 MOTA 1628 CA LEU 232 16.446 8.522 39.675 1.000 12.47 ANISOU 1628 CA LEU 232 1880 1203 -169 4 5 1657 109 1629 CB LEU 232 14.950 8.214 39.552 1.000 12.81 MOTA LEU 232 14.950 8.214
LEU 232 1989 1225
LEU 232 14.452 7.464
LEU 232 2171 1753
1 LEU 232 15.020 6.055
1 LEU 232 2693 1749
2 LEU 232 12.914 7.411
2 LEU 232 2180 1866
LEU 232 16.964 9.354 ANISOU 1629 CB 1654 -209 1 9 -78 1630 CG 38.314 1.000 14.85 MOTA ANISOU 1630 CG 1719 -5 -410 - 96 1631 CD1 LEU 38.240 1.000 16.78 ANISOU 1631 CD1 LEU 1932 72 - 431 - 487 38.291 1.000 15.70 1632 CD2 LEU ANISOU 1632 CD2 LEU -278 -589 4 9 4 1920 1633 C 38.511 1.000 11.58 MOTA 232 1452 ANISOU 1633 C LEU 1390 1559 309 -301 1 3 6 LEU 232 17.752 8.837 37.686 1.000 13.45 1634 O MOTA ANISOU 1634 O LEU 232 1808 1436 -17 3 0 1867 320 1635 N VAL 233 16.565 10.617 38.414 1.000 10.95 MOTA ANISOU 1635 N VAL 233 1428 1210 1522 -14 -210 0 1636 CA VAL 233 16.948 11.421 37.242 1.000 11.70 MOTA ANISOU 1636 CA VAL 233 1703 1397 975 1 3 1345 VAL 233 16.156 12.743 37.215 1.000 11.14 1637 CB ANISOU 1637 CB VAL 233 1672 1272 1287 -26 276 7 3 1638 CG1 VAL 233 16.661 13.774 38.249 1.000 13.34 ANISOU 1638 CG1 VAL 233 1834 1562 1673 -205 653 -368 1639 CG2 VAL 233 16.106 13.412 35.827 1.000 14.66 ATOM ANISOU 1639 CG2 VAL 233 1992 1873 1704 -4 -45 5 8 6 ATOM 1640 C VAL 233 18.459 11.586 37.132 1.000 13.41 1640 C VAL 233 1712 1573 1811 91 151 1 2 5 1641 O VAL 233 19.012 11.627 36.021 1.000 13.45 ANISOU 1640 C MOTA VAL 233 1844 1402 1866 46 192 4 3 8 THR 234 19.188 11.665 38.250 1.000 13.13 ANISOU 1641 O MOTA 1642 N ANISOU 1642 N THR 1643 CA ATOM THR 234 1483 234 21.069 234 1300 1600 1855 -188 428 1 4 3 12.726 39.465 1.000 12.46 1632 1803 -32 200 2 5 1 11.941 40.639 1.000 13.71 ANISOU 1643 CA THR 1644 CB ATOM THR ANISOU 1644 CB THR 1645 OG1 THR 234 20.825 ATOM ANISOU 1645 OG1 THR 234 1660 1662 192 202 291 1888 1662 1888 192 202 2 14.027 39.643 1.000 11.37 234 20.301 MOTA 1646 CG2 THR 234 1097 1565 1657 -153 -87 1 234 21.424 10.643 38.178 1.000 14.44 234 1550 1823 2114 6 -73 - 5 3 1657 -153 -87 169 ANISOU 1646 CG2 THR 1647 C THR ATOM ANISOU 1647 C THR 234 1550

						- 144 -		
ATOM	164	8 0	THR		4 22.659	10.710	38.233	1.000 15.81
ANISO			THR		1 1546	2169	2293	61 27 21 7
ATOM	164		GLY		5 20.767	9.477	38.070	1.000 14.76
ANISO			${ t GLY}$		5 1776	1576	2254	-77 81 410
ATOM	165	0 CA	${ t GLY}$	235	5 21.530	8.249	37.994	1.000 16.69
ANISO	J 1650	O CA	${ t GLY}$	235	2053	1803	2486	
ATOM	165		${ t GLY}$	235	5 22.243	7.862	39.275	304 35 1 8 9 1.000 16.83
ANISO			GLY	235	1854	2031	2512	
ATOM	1652		${ t GLY}$	235	23.305	7.237	39.194	765 244 193 1.000 19.67
ANISO			${ t GLY}$	235	2074	2172	3225	
ATOM	1653		${ t GLY}$	236	21.665	8.227	40.425	1035 383 372
ANISOU			${ t GLY}$	236	1732	1327	2433	
ATOM	1654	CA	${ t GLY}$	236	22.187	7.768	41.692	154 198 7 5 1.000 15.73
ANISOU			GLY	236	2060	1381	2536	41 186 3 1 2
ATOM	1655	C	GLY	236	23.166	8.691	42.388	1.000 14.76
ANISOU			GLY	236	1931	1332	2346	252 73 2 8 8
ATOM ANISOU	1656		GLY	236	23.778	8.244	43.373	1.000 18.32
ANISOC			GLY	236	1983	2197	2782	106 -105 8 4 4
ANISOU	1657	N	GLN	237	23.318	9.938	41.953	1.000 13.99
ATOM	1650	N	GLN		1831	1349	2137	158 165 170
ANISOU	1658	CA	GLN	237	24.209	10.956	42.485	1.000 13.13
ATOM			GLN	237	1474	1304	2210	367 -31 276
ANISOU	1659	CB	GLN	237	24.629	11.948	41.383	1.000 13.38
ATOM	1660		GLN	237	1367	1566	2151	99 72 1 5 9
ANISOU	1660	CG	GLN	237	25.390	11.335	40.219	1.000 14.74
ATOM	1661		GLN	237	1404	1529	2666	518 410 333
ANISOU	1661	CD	GLN	237	25.816	12.428	39.257	1.000 17.22
ATOM	1662	OF1	GLN GLN	237	2039	2018	2486	-64 426 360
ANISOU	1662	OEI	CLN	237	26.754	13.208	39.522	1.000 20.60
ATOM	1663	MES	CIN	23/	1566	2334	3928	-10 -29 965
ANISOU	1663	MES	CIM	23/	25.116	12.470	38.127	1.000 17.47
ATOM	1664	C	GLN	237	2014	2093	2533	208 438 408
ANISOU	1664	Č	GLN	23/	23.627 1474	11.739	43.663	1.000 12.90
ATOM	1665		GLN		24.332	1324	2104	72 -10 255
ANISOU	1665	Ō	GLN	237	1739	12.549	44.282	1.000 15.90
ATOM	1666	N	VAL		22.365	1888	2413	-291 74 - 84
ANISOU	1666	N	VAL		1372	11.481	44.013	1.000 12.13
ATOM	1667	CA	VAL	238	21.664	962 22		
ANISOU	1667	CA	VAL		1169	12.182 1436	45.082	
MOTA	1668	CB	VAL	238	20.622	13.158	1920	-121 -276 - 19
ANISOU	1668	CB	VAT.	238	1024	1179		1.000 12.00
MOTA	1669	CG1	VAI.		19.978	13.999	2357	-6 199 - 3 1
ANISOU	1669	CG1	VAL	238	1530	1668	45.601	1.000 13.07
ATOM	1670	CG2	VAT.	238	21.207	14.088	1767	63 -232 -222
ANISOU	1670	CG2	VAL	238	1795	1470	43.463 2053	1.000 14.00
ATOM	1671	С	VAL	238	20.990		46.000	-40 -2 1 8 1
ANISOU			VAL	238	1707	1415	2054	1.000 13.62
MOTA	1672	0	VAL	238	20.252	10.288	45.492	-103 -40 - 22
ANISOU	1672	0	VAL	238	1702	977 212		1.000 12.64 -318 257
ATOM	1673	N	LYS	239	21.247	11.246	47.300	
ANISOU			LYS	239	1075	1404	2076	1.000 11.99
ATOM	1674	CA	LYS	239	20.568	10.444	48.322	127 -101 7 4
ANISOU			LYS	239	1224	1541	2088	1.000 12.77 -12 -124 8 6
ATOM	1675	CB	LYS	239	21.382	10.463		-12 -124 8 6 1.000 12.23
ANISOU			LYS	239	1333	1155	2158	
ATOM	1676	CG	LYS	239	20.953	9.626	50.793	183 -234 - 28 1.000 13.85
ANISOU	10/6	CG	LYS	239	1643	1689	1931	187 -52 - 8 9
ATOM	1677	CD	LYS	239	21.927	9.579		1.000 20.13
ANISOU ATOM			LYS	239	2893	1795	2961	10 -1185 5 8 8
AIUM	1678	CE	LYS	239	21.364	8.745	53.098	1.000 24.73

- 145 -ANISOU 1678 CE LYS 239 4065 2250 3080 -348 -1465 1064 239 22.019 8.841 54.420 1.000 3-2.28 239 5658 4315 2293 1610 -930 -1679 NZ LYS ANISOU 1679 NZ LYS 1610 -930 - 304 1680 C LYS 239 19.169 10.949 48.661 1.000 11.59 ANISOU 1680 C LYS 239 1207 1332 1866 -35 -82 6 4 1681 0 LYS 239 18.976 12.191 48.708 1.000 12.32 MOTA LYS 239 1638 1294 1749 -2 -25 2 3 6

ALA 240 18.222 10.047 48.863 1.000 10.65

ALA 240 1248 1266 1534 -52 -185 - 8 8

ALA 240 16.884 10.368 49.354 1.000 10.21

ALA 240 1292 1057 1531 -195 -37 -10:

ALA 240 15.784 9.782 48.466 1.000 13.46

ALA 240 1195 2378 1543 -232 20 -403 ANISOU 1681 O 1682 N MOTA ANISOU 1682 N MOTA 1683 CA ANISOU 1683 CA -195 -37 -109 1684 CB ALA 240 1195 2378 1543 -232 20 -40
ALA 240 16.784 9.881 50.807 1.000 10.97
ALA 240 1308 1249 1611 -127 -1424
ALA 240 16.595 8.664 51.059 1.000 13.02 ANISOU 1684 CB 1685 C ATOM ANISOU 1685 C -127 -142 4 9 1686 0 MOTA ANISOU 1686 O ALA 240 2136 1242 1568 -243 28 - 7 ATOM 1687 N PRO 241 16.967 10.783 51.782 1.000 11.13 160 ANISOU 1687 N PRO 241 1723 1041 1466 -49 138 PRO 241 17.172 12.237 51.654 1.000 11.17 ATOM 1688 CD ANISOU 1688 CD PRO 241 1419 1204 1618 -180 -128 7 6 1689 CA PRO 241 17.043 10.340 53.166 1.000 11.96 MOTA 1447 1499 ANISOU 1689 CA PRO 241 1597 -172 -32 193 241 1875 1837 1701 -531 -383 2 4 17.286 12.724 53.069 1.000 13.61 241 2015 1446 1709 -596 -465 - 241 15.708 10.072 53.861 1.000 12.35 241 1417 1610 1665 -175 -187 4 241 14.759 10.829 53.655 1.000 12.28 241 1359 1582 1723 -232 -468 0 1690 CB PRO 241 17.712 11.545 53.891 1.000 14.25 MOTA ANISOU 1690 CB PRO 241 1875 -531 -383 2 4 2 PRO 1691 CG MOTA ANISOU 1691 CG -596 -465 - 22 PRO 1692 C PRO MOTA ANISOU 1692 C PRO -187 4 1 8 1693 O MOTA PRO ANISOU 1693 O 241 1359 1582 1723 -232 -468 8 242 15.700 9.033 54.711 1.000 12.75 PRO -232 -468 8 1 1694 N ARG ATOM 1407 242 1775 -170 76 2 5 0 ANISOU 1694 N ARG 1664 242 14.563 8.804 55.576 1.000 10.76 1695 CA ARG ATOM ANISOU 1695 CA ARG 242 1292 1417 1380 -207 -281 2 1 1 1696 CB ARG 242 14.614 7.405 56.223 1.000 15.02 1696 CB ARG 242 2419 1368 1918 -357 117 2 MOTA -357 117 294 ANISOU 1696 CB ARG 242 14.115 6.342 55.230 1.000 17.85 1697 CG ARG ATOM ANISOU 1697 CG ARG 242 3373 1274 2135 9 -560 253 ATOM 1698 CD ARG 242 14.254 4.934 55.763 1.000 19.42 ANISOU 1698 CD ARG 242 3148 1111 3120 506 503 1 9 -560 251 503 116 ATOM 1699 NE ARG 242 15.667 4.552 55.849 1.000 20.71 ANISOU 1699 NE ARG 242 3225 2107 2538 938 638 212 ARG 242 16.107 3.444 56.416 1.000 23.22 1700 CZ MOTA ANISOU 1700 CZ ARG 242 3198 2206 3417 307 -544 5 8 9 ATOM 1701 NH1 ARG 242 15.285 2.567 56.980 1.000 24.46 ANISOU 1701 NH1 ARG 242 4097 2112 3083 307 387 1 9 5 ATOM 1702 NH2 ARG 242 17.416 3.184 56.438 1.000 25.41 

 242
 17.410
 33.184
 36.438
 1.000
 23.41

 242
 3402
 2332
 3921
 819
 -267
 4

 242
 14.477
 9.834
 56.704
 1.000
 11.95

 242
 1571
 1463
 1506
 -248
 -214
 1

 242
 15.469
 10.377
 57.213
 1.000
 13.65

 242
 1708
 1439
 2040
 -322
 -401

 243
 13.252
 10.085
 57.118
 1.000
 11.60

 ANISOU 1702 NH2 ARG 3921 819 -267 4 0 3 MOTA 1703 C ARG ANISOU 1703 C 1506 -248 -214 1 0 7 ARG 1704 0 MOTA ARG ANISOU 1704 O -322 -401 - 38 ARG 1705 N ATOM HIS ANISOU 1705 N 243 1657 1410 1342 -311 -206 5 HIS 243 12.942 11.056 58.158 1.000 11.49 MOTA 1706 CA HIS ANISOU 1706 CA HIS 243 1855 1571 938 -306 -183 140 243 12.968 12.462 57.546 1.000 11.22 MOTA 1707 CB HIS ANISOU 1707 CB -231 -221 3 9 HIS 243 1432 1379 1453 243 12.133 12.694 56.341 1.000 11.80 1708 CG HIS 243 1937 1171 1378 ANISOU 1708 CG HIS -31

						- 146 -		
MOTA	1709	CD2	HIS	243	10.885	13.236	56 181	1.000 11.15
ANISOU	1709	CD2	HIS	243	1990	1106	1142	35 -34-4, 141
ATOM	1710	ND1	HIS		12.538	12.345		1.000 12.29
ANISOU	1/10	NDI	HIS		1670	1606	1395	394 -91 8
ATOM ANISOU	1711	CEI	HIS		11.599	12.653	54.209	1.000 12.59
ATOM	1712	NE 3	HT2		1686	1740	1357	-522 -202 - 253
ANISOU	1712	NFO	HIC		10.585 1612	13.204	54.841	1.000 10.77
ATOM	1713	C	HIS		11.605	1307 10.737	1172	-616 -268 - 36
ANISOU	1713	Ċ	HIS	243	1869	1570	58.812 1308	1.000 12.49 -321 -53 7 3
MOTA	1714	0	HIS		10.807	9.949	58.271	-321 -53 7 3 1.000 12.26
ANISOU			HIS	243	1756	1404	1497	-188 -115 4 7
ATOM	1715		HIS	244	11.352	11.319	59.983	1.000 12.16
ANISOU			HIS		1464	1715	1442	-230 -112 - 32
ATOM ANISOU	1716		HIS		10.138	11.043	60.758	1.000 12.02
ATOM	1717		HIS HIS		1606	1809	1152	-599 -167 - 24
ANISOU	1717	CB	HIS	244	10.255 1655	9.778	61.615	1.000 12.51
ATOM	1718		HIS		11.270	1763 9.810	1334	-19 101 - 47
ANISOU			HIS		2025	1723	62.698 1965	1.000 15.04
ATOM	1719	CD2	HIS		11.276	10.380	63.923	-178 -433 1 5 4 1.000 18.19
ANISOU	1719	CD3	HIS	244	2946	2339	1627	36 -732 297
ATOM	1720	ND1	HIS	244	12.504	9.203	62.662	1.000 19.30
ANISOU	1720	ND1	HIS		2303	2232	2800	229 -708 2 6 6
ATOM ANISOU	1721	CEI	HIS		13.226	9.387	63.731	1.000 22.48
ATOM	1722	MES	HIS		2649	2734	3159	11 -1206 6 5 0
ANISOU	1722	NE2	HIC		12.476 3088	10.120	64.531	1.000 22.33
ATOM	1723	C	HIS		9.780	2895 12.246	2500	-272 -1236 3 8 4
ANISOU	1723	Ċ	HIS		1897	1673	61.613 1549	
ATOM	1724	0	HIS		10.603	13.165	61.798	-362 254 6 7 1.000 13.48
ANISOU			HIS		1800	1726	1595	-283 139 -161
ATOM	1725	N	VAL		8.551	12.245	62.130	1.000 15.26
ANISOU			VAL		1852	1964	1983	-417 232 - 55
ATOM ANISOU	1726	CA	VAL	245	8.090	13.352	62.970	1.000 17.31
ATOM	1727		VAL	245	2108	2442	2026	-125 476 -161
ANISOU	1727	CB	VAL VAL		6.939 2094	14.169	62.360	1.000 17.33
ATOM	1728		VAL.		6.551	2473	2019	-80 340 -477
ANISOU	1728	CG1	VAL	245	2217	15.334 2966	63.286 4410	1.000 25.25
MOTA	1729	CG2	VAL	245	7.252	14.713	60.966	-137 1939 - 1248 1.000 21.49
ANISOU	1729	CG2	VAL		3070	2538		-180 313 271
ATOM	1730		VAL	245	7.682	12.768	64.327	1.000 18.29
ANISOU			VAL		2123	2689	2137	-443 508 - 71
ATOM	1731		VAL		6.765		64.429	1.000 18.62
ANISOU ATOM			VAL		1810	2174	3089	-15 451 254
ANISOU	1732	N	ALA		8.385	13.202	65.369	1.000 21.54
ATOM	1733		ALA ALA		2813	3045	2327	-591 -407 9 0 7
ANISOU	1733	CA	ALA		8.133 4596	12.701 2562	66.719	1.000 25.10
ATOM	1734		ALA		9.424	12.723	2379	94 - 225 9 9 7
ANISOU	1734	CB	ALA		5381	3408	67.537 2540	1.000 29.82 402 -889 1325
ATOM	1735	С	ALA		7.080	13.545	67.412	1.000 31.20
ANISOU			ALA	246	5079	4143	2632	314 280 428
ATOM	1736	0	ALA	246	6.876	14.714	67.052	1.000 32.39
ANISOU			ALA		4706	3748	3853	567 1247 - 66
ATOM	1737		ALA		6.429	12.973	68.413	1.000 37.30
ANISOU ATOM	1737		ALA	247	5548	5498	3126	92 640 8 3 5
ANISOU	1730	CA	ALA ALA		5.585	13.794	69.271	1.000 40.42
ATOM	1739		ALA		5434 6.289	6048	3878	15 1313 8 5 0
		_		24/	ν. 203	14.132	70.578	1.000 42.17

- 147 -ANISOU 1739 C ALA 247 6495 5891 3636 -823 1720 3 4 1 1740 O 247 7.048 ALA 13.338 71.136 1.000 47.63 ANISOU 1740 O ALA 247 5811 6371 3637 -1631 804 425 1741 CB ALA 247 4.280 13.067 69.525 I.000 47.17 ANISOU 1741 CB ALA 247 5186 9059 3676 -520 523 2683 257 1.781 MOTA 1742 N SER 21.848 70.382 1.000 31.02 ANISOU 1742 N SER 257 4109 5558 2119 137 -235 -810 1743 CA MOTA SER 257 1.214 21.932 69.052 1.000 27.01 ANISOU 1743 CA SER 257 2792 5165 2304 109 -143 - 7071744 CB MOTA SER 257 0.039 22.914 68.992 1.000 28.16 ANISOU 1744 CB SER 257 2655 4473 3572 -238 -90 -1071 1745 OG ATOM SER 257 0.491 24.251 69.074 1.000 51.32 ANISOU 1745 OG SER 257 8516 4131 6853 -616 -2734 -807 1746 C 257 2.259 MOTA SER 22.389 68.034 1.000 26.19 ANISOU 1746 C SER 257 2537 5064 2 3 5.0 -132 -413 -5271747 O ATOM SER 257 3.286 22.988 68.352 1.000 31.47 ANISOU 1747 O 257 2740 SER 5886 3330 -435 -689 -639 1748 N ATOM 258 2..022 ARG 22.123 66.763 1.000 26.04 258 2.982 258 2.982 258 2606 258 2.321 258 2374 ANISOU 1748 N 4477 ARG 2161 -238 -441 - 191749 CA MOTA ARG 22.541 65.747 1.000 25.81 ANISOU 1749 CA ARG 4735 2466 73 -338 -197 1750 C MOTA 22.609 64.383 1.000 18.26 ARG ANISOU 1750 C ARG 2541 2021 39 83 - 854 MOTA 1751 O 258 1.288 21.967 64.131 1.000 19.23 ARG ANISOU 1751 O 258 2600 ARG 2819 -389 311 -4201888 1752 CB 258 4.188 MOTA ARG 21.592 65.664 1.000 29.78 ANISOU 1752 CB 258 3403 ARG 5052 2861 695 -552 - 57ATOM 1753 CG 258 4.246 20.784 64.384 1.000 32.64 ARG ANISOU 1753 CG ARG 258 4358 4148 3896 146 97 - 561 258 5.325 ATOM 1754 CD ARG 19.746 64.499 1.000 30.38 ANISOU 1754 CD 258 3812 ARG 4423 3309 -57 341 - 16 1755 NE 258 6.433 19.909 63.581 1.000 29.43 ATOM ARG ANISOU 1755 NE ARG 258 3990 4604 2588 -22 70 5 4 2 1756 CZ MOTA 19.389 62.359 1.000 25.02 ARG 258 6.453 ANISOU 1756 CZ ARG 258 2540 3893 3074 304 -243 1 0 4 1757 NH1 ARG ANISOU 1757 NH1 ARG 258 2105 2607 3982 359 315 289 1758 NH2 ARG MOTA 258 7.523 19.593 61.617 1.000 22.03 ANISOU 1758 NH2 ARG 258 2477 2775 3120 -430 -287 -964 MOTA 1759 N 23.415 63.527 1.000 20.17 THR 259 2.927 ANISOU 1759 N THR 259 2010 3640 2013 -743 91 -1001 1760 CA 259 2.485 MOTA THR 23.505 62.138 1.000 18.33 ANISOU 1760 CA 259 1801 THR 3043 2121 -533 43 - 685 1761 CB MOTA THR 259 1.821 24.821 61.713 1.000 23.23 ANISOU 1761 CB 3169 THR 259 2082 3576 -384 -164 - 580 259 2.839 25.830 61.681 1.000 34.27 1762 OG1 THR ANISOU 1762 OG1 THR 259 2181 2562 8277 -137 -996 - 794 259 0.738 25.198 62.704 1.000 25.49 MOTA 1763 CG2 THR ANISOU 1763 CG2 THR ATOM 1764 C THR 259 4466 2233 2987 325 396 - 948 259 3.702 23.352 61.222 1.000 18.44 ANISOU 1764 C THR 259 2035 2822 2150 -753 274 -583 259 4.835 1765 O ATOM THR 23.698 61.603 1.000 24.74 ANISOU 1765 O THR 259 1961 5370 2069 -964 231 -714 1766 N MOTA SER 260 3.420 22.867 60.026 1.000 16.29 ANISOU 1766 N SER 260 1971 2352 1864 -224 2 - 75 1767 CA MOTA SER 260 4.447 22.832 58.989 1.000 17.43 ANISOU 1767 CA 260 1783 SER 2961 1879 321 -95 - 721768 CB MOTA SER 260 5.224 21.514 58.956 1.000 20.17 ANISOU 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 1769 OG ATOM SER 260 4.416 20.392 58.698 1.000 27.09 SER 260 3651 ANISOU 1769 OG 2803 3839 426 217

		- 148	_	
ATOM 1770 C	SER 260 3		62 57.614	1.000 14.52
ANISOU 1770 C ATOM 1771 O		1463 2165	1889	83 -160 1
ANISOU 1771 O	SER 260 2 SER 260 1	2.686 22.6		1.000 15.92
ATOM 1772 N	SER 261 4			-93 -1 2 5 7
ANISOU 1772 N	SER 261 1		50 56.742 1788	1.000 13.45
ATOM 1773 CA	SER 261 4			-190 -120 - 500 1.000 13.52
ANISOU 1773 CA	SER 261 1	1726	1812	-204 30 - 315
ATOM 1774 C ANISOU 1774 C	SER 261 5	5.209 22.9	43 54.545	1.000 12.45
ATOM 1775 O	SER 261 1 SER 261 6			-42 $-240$ $-161$
ANISOU 1775 O	SER 261 6 SER 261 1			1.000 15.07
ATOM 1776 CB	SER 261 4			-68 -331 - 343
ANISOU 1776 CB	SER 261 2		2404	1.000 17.76 -399 -485 - 318
ATOM 1777 OG	SER 261 4	.428 25.5		-399 -485 - 318 1.000 27.54
ANISOU 1777 OG ATOM 1778 N	SER 261 4		2814	-719 -821 9 5 5
ANISOU 1778 N	VAL 262 4 VAL 262 1			1.000 10.90
ATOM 1779 CA		215 1630 .393 21.0	1299	41 -135 1 9
ANISOU 1779 CA	VAL 262 1		31 53.026 1442	1.000 11.61 156 -103 1 7
ATOM 1780 CB	VAL 262 5	.026 19.6		156 -103 1 7 1.000 11.87
ANISOU 1780 CB		262 1636	1614	9 -187 - 74
ATOM 1781 CG1 ANISOU 1781 CG1		.778 18.5	_	1.000 13.12
ATOM 1782 CG2	VAL 262 1 VAL 262 5	462 1527 .262 19.5	1997	-2 185 5 1
ANISOU 1782 CG2		390 1494	54 55.062 1604	1.000 17.08
ATOM 1783 C	VAL 262 5	.096 21.1		-374 -245 3 9 1.000 11.18
ANISOU 1783 C ATOM 1784 O	VAL 262 1	026 1790	1431	1 -111 -138
ATOM 1784 O ANISOU 1784 O	VAL 262 3 VAL 262 1		· <b></b> ·	1.000 12.76
ATOM 1785 N	VAL 262 1 PHE 263 6	064 2137 .090 21.43		-251 -84 -271
ANISOU 1785 N	PHE 263 9	95 1297		1.000 9.50 -210 -181
ATOM 1786 CA	PHE 263 5	.933 21.63		1.000 9.61
ANISOU 1786 CA ATOM 1787 CB		310 1017	1324	-6 -284 - 42
ANISOU 1787 CB	PHE 263 6 PHE 263 1			1.000 10.94
ATOM 1788 CG	PHE 263 6			-50 -253 4
ANISOU 1788 CG	PHE 263 7	79 1231	1921 -58	1.000 10.35
ATOM 1789 CD1	PHE 263 6	.858 22.93		1.000 9.98
ANISOU 1789 CD1 ATOM 1790 CD2			1841 -26	-101 240
ANISOU 1790 CD2	PHE 263 5 PHE 263 1:			1.000 11.95
ATOM 1791 CE1	PHE 263 6		2052	245 -29 261 1.000 12.49
ANISOU 1791 CE1	PHE 263 1	718 1173	<del>-</del>	31 -370 136
ATOM 1792 CE2		.769 24.60		1.000 13.12
ANISOU 1792 CE2 ATOM 1793 CZ			2151	43 - 292 353
ANISOU 1793 CZ	PHE 263 5 PHE 263 1:	.491 24.13 318 1453		1.000 12.42
ATOM 1794 C	PHE 263 6			-138 -187 6 4 9 1.000 8 . 9 1
ANISOU 1794 C	PHE 263 1	076 1085		-39 -142 2 4
ATOM 1795 O ANISOU 1795 O	PHE 263 7	.868 20.40	6 48.538	1.000 10.98
ATOM 1796 N	PHE 263 10 PHE 264 5		1842	-120 -224 - 145
ANISOU 1796 N	PHE 264 5 PHE 264 1	.856		1.000 9.19
ATOM 1797 CA	PHE 264 6	.386 18.60		-86 -105 - 82 1.000 9.64
ANISOU 1797 CA	PHE 264 1	009 1238		-56 -60 -126
ATOM 1798 CB ANISOU 1798 CB	PHE 264 5	.483 17.39	8 47.005	1.000 9.92
ATOM 1799 CG	PHE 264 1: PHE 264 5		1359	-78 17 9
ANISOU 1799 CG	PHE 264 1:	.265 16.61 241 1647		1.000 11.22
ATOM 1800 CD1	PHE 264 6	.292 16.23		-121 38 7 7 1.000 15.38
				000 , J , J 0

- 149 -ANISOU 1800 CD1 PHE 264 1467 264 3.988 2641 1734 -225 -8873 1801 CD2 PHE 16.433 48.808 1.000 16,96 3252 1769 -610 -79 958 ANISOU 1801 CD2 PHE 264 1425 3252 1769 -610 -79 9 264 6.090 15.596 50.336 1.000 14.52 1802 CE1 PHE ANISOU 1802 CE1 PHE 2417 1354 162 334 452 1803 CE2 PHE 264 3.755 15.796 50.019 1.000 18.04 ANISOU 1803 CE2 PHE 264 1747 3405 1704 -590 -109 1807 ATOM 1804 CZ PHE 264 4.817 15.354 50.779 1.000 12.55 ANISOU 1804 CZ PHE 264 1772 1536 1449 -57 227 38 ANISOU 1805 C PHE 264 6.535 19.038 45.533 1.000 8.98 ANISOU 1805 C PHE 264 1103 919 1392 143 81 -92 ATOM 1806 O PHE 264 5.497 19.368 44.930 1.000 9.79 ANISOU 1806 O PHE 264 991 1190 1540 28 105 103 ANISOU 1806 O PHE 264 991 1190 1540 28 105 103 ANISOU 1803 CE2 PHE 264 1747 -590 -109 1 0 0 8 15.354 50.779 1.000 12.52 1536 1449 -57 227 334 19.038 45.533 1.000 8.98 ATOM 1807 N LEU 265 7.758 19.031 44.999 1.000 8.43
ATOM 1807 N LEU 265 992 884 1325 173 -180 158
ATOM 1808 CA LEU 265 7.984 19.224 43.566 1.000 8.66
ANISOU 1809 CB LEU 265 9.309 19.964 43.328 1.000 10.10
ANISOU 1809 CB LEU 265 1179 1188 1469 -225 -220 2 4 8
ANISOU 1809 CB LEU 265 1179 1188 1469 -225 -220 2 4 8
ANISOU 1810 CG LEU 265 9.570 20.351 41.871 1.000 9.37
ANISOU 1811 CD1 LEU 265 8.725 21.522 41.408 1.000 10.80
ANISOU 1811 CD1 LEU 265 1291 1004 1811 181 -114 2 9 6
ATOM 1812 CD2 LEU 265 1129 1483 1519 134 43 1 4 6
ANISOU 1813 C LEU 265 7.933 17.849 41.678 1.000 10.21
ANISOU 1813 C LEU 265 7.933 17.849 48.75 1.000 10.21
ANISOU 1814 O LEU 265 8.858 17.043 43.042 1.000 10.21
ANISOU 1815 N ARG 266 6.853 17.530 42.135 1.000 10.45
ANISOU 1815 N ARG 266 6.853 17.530 42.135 1.000 10.00
ANISOU 1816 CA ARG 266 1325 1069 1404 -120 -222 1 5
ANISOU 1817 CB ARG 266 5.208 15.675 42.124 1.000 10.56
ANISOU 1818 CG ARG 266 1337 1373 1563 -40 119 2 0 6
ANISOU 1818 CG ARG 266 4.965 15.894 43.609 1.000 11.24
ANISOU 1818 CG ARG 266 1337 1373 1563 -40 119 2 0 6
ATOM 1818 CG ARG 266 1337 1373 1563 -40 119 2 0 6
ATOM 1818 CG ARG 266 1337 1373 1563 -40 119 2 0 6
ATOM 1818 CG ARG 266 1337 1373 1563 -40 119 2 0 6 1807 N LEU 265 7.758 19.031 44.999 1.000 8.43 1819 CD ARG 266 3.668 ATOM 15.318 44.146 1.000 11.17 ANISOU 1819 CD ARG 266 1113 1567 ATOM 1820 NE ARG 266 2.508 15.879 43.447 1.000 9.43 ANISOU 1820 NE ARG 266 1341 1157 1086 24 -100 -145 ATOM 1821 CZ ARG 266 1.236 15.509 43.657 1.000 9.83 1564 -17 -49 -11 1821 CZ ARG 266 1245 1194 1294 132 -159 - 1 1822 NH1 ARG 266 0.961 14.567 44.572 1.000 11.20 ANISOU 1821 CZ ATOM ANISOU 1822 NH1 ARG 266 1208 1240 1806 -144 -454 2 ATOM 1823 NH2 ARG 266 0.225 16.048 42.975 1.000 11.08 -144 -454 2 7 2 ANISOU 1823 NH2 ARG 266 1460 1265 1484 191 -283 7 3
ATOM 1824 C ARG 266 6.601 16.190 40.099 1.000 10.28 ANISOU 1824 C ATOM 1825 O ANISOU 1825 O ARG 266 1273 1089 1545 -200 -5 -16 ARG 266 6.027 17.109 39.519 1.000 11.05 -200 -5 -167 ATOM 1825 O ARG 266 6.027 17.109 39.519 1.000 11.05
ANISOU 1825 O ARG 266 1254 1153 1793 -132 47 - 64
ATOM 1826 N PRO 267 7.215 15.162 39.496 1.000 10.27
ANISOU 1826 N PRO 267 1194 1239 1468 -33 130 3
ATOM 1827 CD PRO 267 7.828 13.963 40.109 1.000 12.36
ANISOU 1827 CD PRO 267 1865 1132 1697 -26 -529 -1
ATOM 1828 CA PRO 267 7.304 15.157 38.036 1.000 10.12
ANISOU 1828 CA PRO 267 1278 1095 1472 -129 38 -18
ANISOU 1829 CB PRO 267 8.250 13.986 37.767 1.000 11.83
ANISOU 1829 CB PRO 267 8.250 13.986 37.767 1.000 11.83
ATOM 1830 CG PRO 267 8.017 13.053 38.913 1.000 10.72
ANISOU 1830 CG PRO 267 960 1356 1755 95 -257 -187 -132 47 - 64 -33 130 3 2 -26 -529 - 192 -129 38 - 185 90 - 322

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ATOM	1831	С	PRO	267	5.977	14.929	37.344	1.000 10.86
ANISOU	1831	С	PRO	267	1330	1226	1570	-252- <del>1</del> 7, -161
ATOM	1832	0	PRO	267	5.030	14.421	37.934	1.000 12.03
ANISOU		0	PRO	267	1316	1174	2080	~-258 17 7 7
ATOM	1833	N	ASN	268	5.931	15.288	36.065	1.000 10.61
ANISOU		N	ASN	268	1216	1146	1670	-70 -86 -129
ATOM	1834		ASN	268	4.810	14.949	35.198	1.000 11.20
ANISOU			ASN	268	1285	1349	1622	-167 -43 -229
ATOM ANISOU	1835	CB	ASN	268	4.954	15.664	33.846	1.000 14.02
ANISOU	1836	CG	ASN ASN	268	2160	1410	1756	132 -316 2 3
ANISOU			ASN	268 268	4.992 1811	17.175	33.992	1.000 13.03
ATOM	1837	OD1		268	4.046	1393 17.748	1747 34.566	189 -355 - 88
ANISOU		OD1		268		1744	2673	1.000 16.65 292 -1 - 159
ATOM	1838	ND2		268	6.037	17.818	33.495	1.000 14.19
ANISOU	1838	ND2	ASN		2505	1372	1516	161 264 -172
ATOM	1839	С	ASN		4.705	13.446	34.968	1.000 10.88
ANISOU		С	ASN	268	1294	1314	1526	-75 -226 - 164
ATOM	1840	0	ASN	268	5.715	12.732	34.979	1.000 11.68
ANISOU		0	ASN	268	1534	1439	1464	87 -458 -121
ATOM	1841		ALA	269	3.484	12.980	34.688	1.000 12.22
ANISOU ATOM	1841	N	ALA	269	1484	1428	1732	-108 -397 -427
ANISOU		CA CA		.269	3.277	11.547	34.417	1.000 12.12
ATOM	1843	CB	ALA ALA	269 269	1432 1.817	1356	1819	-238 -29 -282
ANISOU		CB	ALA	269	1439	11.310 1278	34.058 1985	1.000 12.38
ATOM	1844	C	ALA		4.125	10.981	33.283	-228 -183 2 9 1.000 11.26
ANISOU		Č	ALA	269	1445	1240	1592	25 - 280 - 141
ATOM	1845	0	ALA	269		9.800	33.263	1.000 12.53
ANISOU		0	ALA	269	1428	1249	2085	-110 108 -188
ATOM		N	ASP		4.438	11.799	32.276	1.000 11.47
ANISOU		N	ASP		1701	1280	1378	-261  -341  -300
ATOM	1847		ASP		5.214	11.378	31.113	1.000 11.92
ANISOU		CA	ASP		1826	1106	1595	19 -183 -156
ATOM	1848	CB	ASP		4.760	12.096	29.850	1.000 14.13
ANISOU ATOM	1849	CB CG	ASP ASP		1733	2038	1597	84 111 2 1 2
ANISOU		CG	ASP	270	5.050 2309	13.568	29.777	1.000 15.98
ATOM	1850	OD1			5.432	1939 14.186	1823 30.762	418 -418 5 6 4
ANISOU		OD1				1797	2312	1.000 21.61 176 -515 1 6 3
ATOM	1851	OD2			4.880	14.152	28.674	1.000 24.64
ANISOU		OD2			3995	3221	2145	-62 -169 1 3 9 5
ATOM	1852		ASP		6.721	11.542	31.264	1.000 12.86
ANISOU		С	ASP	270	1840	1392	1654	-398 -61 315
MOTA	1853	0	ASP		7.443	11.290	30.292	1.000 14.83
ANISOU		0	ASP		1813	2114	1709	-346 -141 4 9
ATOM	1854		PHE		7.230	11.911	32.439	1.000 11.85
ANISOU			PHE		1360	1316	1824	59 -25 7 0
ATOM	1855		PHE		8.665	11.927	32.715	1.000 11.14
ANISOU ATOM	1856	CB	PHE PHE		1242	1349	1641	10 230 1 6 2
ANISOU		CB	PHE		8.972 1467	12.378	34.143	1.000 12.19
ATOM	1857		PHE		10.385	1444 11.992	1722	-96 -3 1 8 2
ANISOU			PHE		1411	1640	34.597 1800	1.000 12.77 42 31 5 6
ATOM	1858				11.475	12.488	33.904	1.000 13.22
ANISOU				271	1513	1516	1993	168 220 4 9
ATOM	1859	CD2	PHE		10.624	11.155	35.666	1.000 13.55
ANISOU	1859	CD2	PHE		1343	1674	2131	139 84 2 5 5
MOTA	1860	CE1	PHE	271	12.779	12.178	34.249	1.000 14.26
ANISOU				271	1432	1760	2225	-39 46 - 416
ATOM	1861	CE2	PHE:	271	11.925	10.806	36.019	

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	1061					- 151 -		
ANISOU ATOM	1861				1537	1818	2679	-263 -675 2 6 0
ANISOU			PHE PHE		13.006	11.288		
ATOM	1863		PHE	271	1166 9.259	1736	2475	7 -531 -467
ANISOU			PHE	271	1359	10.550 1338	32.410	1.000 11.27
ATOM	1864		PHE		8.785	9.531	1585 32.920	75 271 3 4 8
ANISOU			PHE	271		1320	1596	1.000 12.97 -85 473 279
ATOM	1865		THR	272	10.261	10.498	31.541	-85 473 279 1.00011.95
ANISOU			THR	272	1018	1503	2020	-214 300 -115
MOTA	1866	CA	THR		10.823	9.254	30.992	1.000 12.70
ANISOU	1866	CA	THR		1615	1557	1652	132 341 146
MOTA	1867		THR	272	10.679	9.281	29.450	1.000 16.79
ANISOU			THR		1814	2829	1737	-595 157 -406
MOTA	1868		THR		9.301	9.471	29.090	1.000 18.02
ANISOU				272	1912	2921	2013	-497 -73 9 1
ATOM	1869	CG2	THR	272	11.200	7.976	28.856	1.000 17.02
ANISOU					2144	2857	1467	-475 538 -194
ATOM ANISOU	1870		THR		12.272	9.057	31.423	1.000 12.02
ANISOU	1871		THR THR		1436 13.055	1573	1559	92 603 1 3 7
ANISOU			THR	272	13.055	10.031 1583	31.437	1.000 14.17
ATOM		Ŋ	PHE	273	12.625	7.837	2351 31.828	125 602 412
ANISOU			PHE	273	1402	1585	1703	1.000 12.34 17 378 1 5 8
MOTA	1873		PHE		13.953	7.492	32.312	1.000 12.20
ANISOU			PHE	273	1362	1364	1909	-126 336 147
ATOM	1874		PHE	273		7.514	33.861	1.000 12.37
UOZINA			PHE	273	1362	1447	1890	-102 211 - 8
ATOM	1875		PHE		12.988	6.528	34.491	1.000 11.65
ANISOU			PHE	273		1631	1396	-367 42 - 215
ATOM	1876	CD1	PHE	273		6.889	34.773	1.000 14.11
ANISOU					1531	2214	1614	-336 293 - 62
ATOM ANISOU	1877	CD2	PHE		13.409	5.245	34.803	1.000 13.20
ANISOU	1878	CD2	PHE	273 273		1639	1352	-358 339 - 9
ANISOU	1878	CE1	PHE		10.793 1536	5.993	35.323	1.000 13.25
ATOM	1879	CE2	PHE	273		2081 4.329	1418 35.327	-98 447 4 2
ANISOU	1879	CE2	PHE	273	1529	1905	35.327 1654	1.000 13.39 -224 140 283
ATOM	1880		PHE	273	11.227	4.706	35.604	1.000 14.75
ANISOU			PHE	273	1444	2260	1902	-90 -186 2 7 5
ATOM	1881	С	PHE	273		6.135	31.795	1.000 12.45
ANISOU	1881	С	PHE		1278	1526	1927	-120 317 - 31
MOTA			PHE	273	13.645	5.311	31.291	1.000 11.95
ANISOU			PHE		1590	1580	1370	-137 226 - 13
MOTA	1883		SER		15.717	5.854	31.952	1.000 12.07
ANISOU			SER		1270	1640	1677	-29 558 353
ATOM	1884		SER		16.335	4.586	31.604	1.000 14.39
ANISOU			SER		1583	1534	2349	43 707 3 8 4
ATOM ANISOU	1885		SER		17.845	4.771	31.438	1.000 14.49
ATOM	1886		SER SER		1578 18.564	1727	2202	213 695 329
ANISOU			SER		1763	3.558 1848	31.424	1.000 14.97
ATOM	1887	C	SER		16.100	3.505	2078 32.666	349 348 - 13
ANISOU		C	SER		1670	1481	1833	1.000 13.12 8 461 137
ATOM	1888		SER		16.438	3.700	33.834	1.000 13.50
ANISOU			SER		1493	1518	2116	-65 119 1 5
ATOM	1889		VAL		15.533	2.359	32.271	1.000 11.90
ANISOU			VAL		1476	1618	1427	-110 490 195
MOTA	1890		VAL			1.254	33.180	1.000 11.41
ANISOU			VAL	275	1708	1424	1204	-8 286 7 6
ATOM	1891		VAL	275	14.346	0.198	32.543	1.000 12.74
ANISOU	1891	CB	VAL	275	1732	1300	1809	62 164 - 1 6

				- 152 -		
ATOM 1892	CG1 VA		14.157	-1.020	33.437	1.000 16.10
ANISOU 1892	CG1 VA		2352	1803	1962	-614 <b>-663</b> 3 7 0
ATOM 1893	CG2 VA		12.961	0.763	32.261	1.000 13.81
ANISOU 1893 ATOM 1894			1535	1786	1924	16 363 1 2 6
ATOM 1894 ANISOU 1894			16.577	0.622	33.692	1.000 12.62
ATOM 1895			1574	1628	1594	14 375 1 3 6
ANISOU 1895	O VA		16.729	0.405	34.926	1.000 13.01
ATOM 1896			1667	1643	1634	9 118 1 8 0
	N PR		17.569 1583	0.286	32.889	1.000 14.64
ATOM 1897			17.583	2066 0.285	1914	2 454 - 42
ANISOU 1897			1565	2536	31.415 1916	1.000 15.84
ATOM 1898	CA PR		18.827	-0.250	33.453	89 755 3 5 1.000 16.76
ANISOU 1898	CA PR		1667	2403	2296	
ATOM 1899		.0 276	19.732	-0.503	32.236	261 393 - 163 1.000 18.27
ANISOU 1899		.0 276	1804	2568	2571	411 574 -142
ATOM 1900			18.868	-0.385	31.029	1.000 18.96
ANISOU 1900 ATOM 1901		_	2147	2763	2293	725 694 - 37
ATOM 1901 ANISOU 1901	C PR		19.500	0.710	34.420	1.000 16.32
ATOM 1902			1521	2342	2336	115 237 6 7
	O PR		20.035 1411	0.277	35.456	1.000 16.78
	N LE		19.475	2689	2275	93 376 2 5 3
ANISOU 1903	N LE		1835	2.019	34.155	1.000 16.58
ATOM 1904			20.142	2412 2.919	2052	-15 483 148
ANISOU 1904	CA LE		1990	2226	35.099 2511	1.000 17.70 -21 362 118
ATOM 1905	CB LE		20.298	4.277	34.425	-21 362 118 1.000 20.20
ANISOU 1905			2952	2292	2432	-1 -14 2 7 1
ATOM 1906	CG LE		21.048	5.359	35.186	1.000 20 . 86
ANISOU 1906	CG LE			2221	3490	-32 -355 4 8 2
ATOM 1907	CD1 LE	U 277	22.446	4.888	35.531	1.000 34.24
ANISOU 1907 ATOM 1908	CD1 LE		2157	2303	8552	69 -842 258
ANISOU 1908	CD2 LE		21.062	6.620	34.334	1.000 31.91
ATOM 1909	CD2 LE		4745	2460	4918	-474 -572 1 1 5 0
ANISOU 1909	C LE		19.411 1975	2.989	36.430	1.000 16.55
ATOM 1910			19.997	1885 3.116	2430	-218 211 -243
ANISOU 1910	O LE		2179	2636	37.517 2476	1.000 19.19
ATOM 1911	N AL		18.080	2.905	36.386	-617 50 1 2 2 1.000 15.48
ANISOU 1911	N AL		2008	1904	1969	-358 279 112
ATOM 1912	CA AL		17.308	2.896	37.636	1.000 14.51
ANISOU 1912	CA AL	A 278	2109	1763		-309 74 1 6 7
ATOM 1913			15.814	2.896	37.347	1.000 15.41
ANISOU 1913			2017	1773	2064	66 301 6 2 6
ATOM 1914 ANISOU 1914			17.710	1.684	38.479	1.000 14.55
ATOM 1915			1972	1869	1689	-195 -255 7 9
ANISOU 1915			17.894	1.770	39.683	1.000 13.80
ATOM 1916			1444 17.841	2144	1655	-250 -166 8 9
ANISOU 1916			17.841	0.530	37.842	1.000 13.86
ATOM 1917			18.242	1728 -0.679	1742	-432 -128 1 6 9
ANISOU 1917	CA AR	G 279	1995	1973	38.560 2064	1.000 15.88 59 355 4 1 1
ATOM 1918	CB AR	G 279	18.204	-1.922	37.648	1.000 16.83
ANISOU 1918	CB AR	G 279	1889	1897	2609	84 544 2 5 0
ATOM 1919		G 279	16.790	-2.323	37.291	1.000 19.63
ANISOU 1919		G 279	2123	2196	3139	-63 233 9 1
ATOM 1920	_		16.656	-3.288	36.131	1.000 27.03
ANISOU 1920 ATOM 1921			3924	3198	3150	-603 -275 - 198
ATOM 1921 ANISOU 1921			17.236	-4.578	36.364	1.000 27.45
ATOM 1922	NE AR		4659	2854	2915	-359 751 - 789
	CL AR	G 219	16.714	-5.717	36.779	1.000 32.85
	_					



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ANISOU	_		ARG	279	4486	3045	4948	-475 448 -222
ATOM	1923				15.424	-5.874	37.089	
ANISOU					4653	2168	4562	-103 967 -678
ATOM	1924				17.551	-6.750	36.890	
ANISOU					4879	2436	7074	-276 3278 - 824
ATOM	1925		ARG		19.628	-0.519	39.150	
ANISOU			ARG		2118	1653	2871	75 -8 7 0 5
ATOM ANISOU	1926		ARG		19.916	-1.064	40.212	1.000 26.82
ANISOU	1927		ARG GLU		3764 20.538	3102	3325	-1987 -1467 1383
ANISOU			GLU		1983	0.189	38.505	
ATOM	1928		GLU		21.899	2293 0.317	2459 39.026	109 609 3 7
ANISOU			GLU		2049	2023	3396	
ATOM	1929		GLU		22.836	0.886	37.936	125 215 737 1.000 20.17
ANISOU			GLU		1648	2457	3560	464 138 1099
ATOM	1930		GLU		22.964	-0.149	36.818	1.000 31.79
ANISOU			GLU		3477	4175	4427	801 1187 - 4
ATOM	1931	CD	GLU		23.698	0.341	35.590	
ANISOU			GLU		5144	5703	4221	-64 1339 - 6
ATOM	1932				24.466	1.327	35.685	
NISOU					3464	5891	5710	334 574 1639
ATOM	1933				23.489	-0.294		1.000 41.55
ANISOU					5257	6747	3781	2245 -184 1 0 2
ATOM	1934		GLU		21.984	1.188	40.266	
ANISOU			GLU		1488	2350	3640	-566 162 490
ATOM	1935		GLU		23.031	1.142	40.958	
ANISOU ATOM	1935		GLU		1871	3766	4123	231 -245 1 8 0
ANISOU			CYS		20.943	1.980	40.565	
ATOM	1937		CYS CYS		1560 21.098	2609	2887	
ANISOU			CYS		3222	2.762 2647	41.806	
ANTSOO	1938		CYS		21.079	4.264	3184 41.523	-1189 176 - 122 1.000 25.40
ANISOU			CYS		3278	2655	3718	-426 368 - 46
ATOM	1939		CYS		19.587	4.904	40.763	1.000 27.05
ANISOU			CYS		3069	2914	4295	-522 -37 -794
ATOM	1940		CYS		20.098	2.406	42.907	1.000 16.99
ANISOU			CYS		1377	1604	3475	109 -6 -546
ATOM	1941	0	CYS		19.971	3.173	43.889	1.000 17.04
ANISOU	1941	0	CYS	281	2294	1277	2902	-204 -484 - 129
ATOM	1942		GLY		19.447	1.245	42.794	1.000 15.23
ANISOU			${ t GLY}$		1617	1597	2572	3 -58 - 436
MOTA	1943		$\mathtt{GLY}$		18.731	0.674	43.914	
ANISOU					1565			6 -331 -266
ATOM			GLY		17.246	0.519	43.727	1.000 13.75
ANISOU			GLY		1635	1562	2029	-270 -446 - 78
ATOM	1945		GLY		16.585	0.012		1.000 14.99
ANISOU			GLY		1751	1630	2313	
ATOM ANISOU	1946		PHE		16.744	1.009	42.582	
ATOM	1945		PHE		1434	1803	1570	-200 18 -252
ANISOU			PHE		15.292	0.886	42.3/4	1.000 11 . 80
ATOM	1947		PHE PHE		1477 14.839	1032	19/4	-15 -264 4 6 1.000 14.13
ANISOU			PHE		2262	972 21	$\frac{41.295}{36}$	9 -187 159
ATOM	1949		PHE		14.906	3.351	.JU .LU	1.000 12.63
ANISOU			PHE		1711	1033	2055	47 -86 9
ATOM	1950				13.851	3.928	42.409	1.000 13.45
ANISOU					1697	1399	2013	
ATOM			PHE		16.037	4.111	41.519	
ANISOU					1567	1135	2295	142 -41 -99
MOTA	1952	CE1	PHE		13.903	5.248	42.839	
ANISOU	1952	CE1	PHE	283	2111	1649	2171	-202 484 -617
					_	-	· <del>-</del>	

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ATOM	195	3 CE	2 PHE	283	3 16.112	5.432	41.963	1 000		
ANISO	U 195	3 CE		283	1783	937 20	91.903 068 32	1.000	12.60	
ATOM	195	4 CZ	PHE	283	15.040	5.993	42.641	10 1	13.37	
ANISON ATOM			PHE	283		865 23	352 18	71	49 1 3	
ANISO	195	5 C	PHE	283		-0.534	41.972	1.000	11 22	
ATOM	195	5 0	PHE	283	1527	9/4 1/	765 63	-172	6 5	
ANISO	1 1 9 5 <i>i</i>	5 0	PHE	283	15.471	-1.071	40.990		13.24	
ATOM	1951	7 N	PHE ASP	283	1249	1428	2355	175	-120 -	3 6 1
ANISO	J 1951	7 N	ASP	284	13.998 1607	-1.130	42.712		12.31	<b>5</b>
ATOM	1958	CA	ASP	204	13.589	1333		-268	-312 8	7
ANISOU	J 1958	3 CA	ASP	284	1725	-2.528 1202	42.527	1.000	12.48	
ATOM	1959	CB	ASP	284	13.159	-3.156	1814		-543 3	5 0
ANISOU	J 1959	CB	ASP	284	2014	1145	43.876 1656		12.67	
ATOM	1960	) CG	ASP		13.261	-4.667	43.909	-50 1 000	-406 1	3 5
ANISOU	1960	CG	ASP	284	2077	1171	1843	110	-4193	
ATOM	1961	OD1	ASP	284	13.861	-5.246	42.974	1 000	1/ 00	6 3
ANISOU ATOM	1067	ODI	ASP	284	1956	1094	2640	-87	11 6 0	
ANISOU	1962	002	ASP	284	12.762	-5.306	44.883	1.000	15.79	
ATOM	1963	C	ASP	284	2494	1539	1966	-330	-446 4 3	3 8
ANISOU	1963	Č	ASP	284	12.478 1238	-2.641	41.510	1.000	10.82	- 0
ATOM	1964	Ŏ	ASP	284	11.373	1387	1487	-205	-99 12	2 3
ANISOU	1964	0	ASP	284	1331	-3.100 1175	41.777	1.000	12.28	
ATOM	1965	N	VAL	285	12.751	1175 -2.154	2159 40.308	-209	48 1 9 1	
ANISOU			VAL	285	1204	1671	1426	-93	11.32	_
ATOM	1966	CA	VAL	285	11.748	-2.062	39.260		-48 6 11.45	1
ANISOU ATOM	1966	CA	VAL	285	1468	1384	1500	39 -21	9 - 15	
ANISOU	1967	CB	VAL	285	12.153	-1.072	38.157	1.000	11.58	
ATOM	1968	CCI	VAL	285	1412	1523	1465		-428 -	R
ANISOU	1968	CGI	VAL	285	12.278	0.362	38.679	1.000	15.02	•
ATOM	1969	CG2	₹ <b>7</b> ΔΤ.	205	2209 13.467	1458	2040	-264	-442 - 3	2
ANISOU	1969	CG2	VAL	285	1909	-1.482	37.495	1.000		
ATOM	1970	C	VAL	285	11.424	1443 -3.431	2615	-159	309 44	. 7
ANISOU	1970	С	VAL	285	1232	1281	38.642 1602	1.000	10.83	
ATOM	1971	0	VAL	285	12.267	-4.301	38.520	93 -22		
ANISOU			VAL	285	1214	1192	2202	1.000 -28		
ATOM	1972	N	SER	286	10.168	-3.523	38.248	1.000	300 16	) 2
ANISOU ATOM	1972	N	SER	286	1116	1608	1489		96 7	
ANISOU	1973	CA	SER	286	9.558	-4.622	37.510	1.000	11.32	
ATOM	1974		SER SER		1104	1479	1718	-41	-274 2 5	2
ANISOU	1974	CB	SER	200	8.483 1328	-5.292	38.344	1.000	9.88	
MOTA	1975	OG	SER	286	7.570	1141	1285	72 -20	770	
ANISOU	1975	OG	SER	286	1391	-4.361 1188	38.905	1.000		
MOTA	1976	С	SER	286	9.019	-4.106	1729 36.175	147	-153 7 !	5
ANISOU	1976	С	SER	286	1127	1227	1575	1.000	10.34	
ATOM	1977	0	SER	286	7.829	-4.112	35.869	28 -87 1.000	245	
ANISOU ATOM	1977	0	SER	286	1223	2219	1353	0 -17	8 228	
ANISOU	1978	N	LEU	287	9.926	-3.622	35.335	1.000	12 15	
ATOM	1979	C 3	LEU	287	1414	1664	1653		3 161	
ANISOU	1979		LEU	287	9.654	-2.900	34.099	1.000		
ATOM	1980		LEU LEU		1622	1558	1605	-366	94 1 8 4	
ANISOU	1980		LEU	201	10.145 1716	-1.452	34.210	1.000	12.91	
ATOM	1981	CG	LEU	287	9.452	1591 -0.590	1597		-95 2 1	7
ANISOU	1981	CG	LEU	287	1182	1848	35.264	1.000		
ATOM	1982	CD1	LEU	287	10.229	0.708	1895 35.484		-51 -1	70
ANISOU	1982	CD1	LEU	287	1644	1108	2318	1.000		2
ATOM	1983	CD2	LEU	287	8.006		_	1.000	-124 2 2 1 4 5 6	3
									. 4	

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ANISCU			LEU	287	1716	1548	2267	36 -550 318
ATOM	1984		LEU	287	10.319		32.928	1.000,-T <sub>2</sub> , 63
ANISCU			LEU		1837	1244	1719	-233 248 354
ATOM ANISOU	1985		LEU	287	11.529	-3.805	32.916	
ANISOU	1986		LEU ASP		1779	1998	2560	-292 390 -149
ANISCU			ASP		9.531 2080	-4.045	31.950	1.000 13.91
ATOM	1987		ASP		10.079	1751 -4.688	1455 30.759	4 223 2 2 7
ANISOU	1987	CA	ASP		2029	2269	1593	1.000 15.50 -122 605 153
ATOM	1988		ASP	288	8.979	-5.478	30.043	-122 605 153 1.000 17.00
ANISOU			ASP		2722	2125	1613	-250 362 - 2
ATOM ANISOU	1989	CG	ASP		9.480	-6.452	29.014	1.000 19.30
ATOM	1990		ASP		2467 10.447	2980	1885	173 243 - 377
ANISOU	1990	ODI	ASP	288	2812	-7.183 3190	29.292 3856	1.000 25.95
ATOM	1991	OD2	ASP		8.911	-6.508	27.907	501 -239 - 783 1.000 31.76
ANISOU	1991	OD2	ASP		5375	4430	2260	1266 -849 -1154
ATOM	1992	C	ASP	288	10.654	-3.652	29.811	1.000 17.08
ANISOU			ASP	288	2259	2631	1602	-263 248 534
ATOM ANISOU	1993		ASP	288	10.197	-2.502	29.708	1.000 23.31
ANISOU	1994		ASP GLY		4276 11.702	2268	2313	-244 -13 297
ANISOU			GLY	289	2748	-3.966 3699	29.049 1632	1.000 21.26
ATOM	1995	CA	GLY		12.116	-2.880	28.152	-610 752 511 1.000 21.65
ANISOU			GLY	289	2842	3988	1396	-1163 71 6 2 6
ATOM	1996	С	GLY	289	13.084	-1.859	28.736	1.000 22.09
ANISOU ATOM	1996		GLY		2888	3509	1996	-738 -23 243
ANISOU			$\operatorname{GLY}$		13.414 3230	-1.836	29.924	1.000 20.34
ATOM	1998		GLU		13.562	2606 -0.952	1891	-918 124 1 4 7
ANISOU	1998	N	GLU		2665	2099	27.869 1496	1.000 16.48 5 222 - 445
MOTA	1999		GLU		14.716	-0.117	28.182	1.000 16.94
ANISOU			GLU		2470	2161	1806	81 411 - 484
ATOM	2000	CB	GLU		15.579	0.012	26.912	1.000 20.26
ANISOU ATOM	2000		GLU		2670	2740	2287	414 863 -239
ANISOU	2001	CG	GLU GLU	290	16.071 3251	-1.333 3153	26.386	1.000 24.53
ATOM	2.002		GLU		16.812	-2.170	2916 27.411	664 1218 - 612 1.000 27.91
ANISOU			GLU		3019	3161	4424	989 940 - 251
ATOM	2003	OE1	GLU	290	17.874	-1.747	27.917	1.000 35.13
ANISOU	2003	OE1	GLU	290	3913	4458	4975	963 -85 -877
ATOM	2004	OE2	GLU		16.336	-3.280		
ANISOU ATOM	2004	C E Z	GLU		6893	3257	6478	-30 -748 5 9 8
ANISOU	2005	C	GLU		14.406 2512	1.271 1756	28.716	1.000 14.67
ATOM	2006	0	GLÜ		15.260	1.840	1308 29.412	95 142 1 0 1.000 15.25
ANISOU	2006	0	GLU		2074	1969	1750	50 418 - 262
ATOM	2007	N	THR	291	13.232	1.814	28.437	1.000 15.72
ANISOU ATOM			THR		2173	2393	1406	78 346 - 519
ANISOU	2008	CA	THR		12.792	3.087	28.991	1.000 15.16
ATOM	2008		THR THR		2080 12.766	1845	1833	-88 631 - 15
ANISOU			THR		2724	4.226 2529	27.956 1842	1.000 18.67
ATOM	2010	OG1	THR		11.756	4.009	26.976	-361 769 3 3 6 1.000 2 2 . 9 3
ANISOU	2010	OG1	THR	291	3313	3135	2265	445 78 1 4 6
ATOM	2011	CG2			14.096	4.306	27.213	1.000 21.82
ANISOU ATOM	2011		THR		3035	2126	3130	357 1450 9 0 2
ANISOU			THR THR		11.402	2.920	29.622	1.000 12.86
ATOM	2012		THR		1863 10.625	1604	1421	47 305 2 1 9
ANISOU			THR	291	2344	2.024 1983	29.270 1804	1.000 16.13
						1703	1004	-303 750 -431

								1 € 17 € 27 € 70 70 70 70 70 70 70 70 70 70 70 70 70
						- 156 <i>-</i>		
ATOM :	2014	N	ALA	292	11.037	3.791	30.542	1.000 12.41
ANISOU 3	2014	N	ALA	292	1495	1363	1859	-2 256 <u>-7</u> 7
ATOM :	2015	CA	ALA	292	9.746	3.839	31.202	1.000 11.57
ANISOU 2	2015	CA	ALA		1362	1257	1779	-213 153 3 7
	2016		ALA		9.718	2.954		
ANISOU 2		CB	ALA		1768	1245	32.439	1.000 12.62
		C	ALA		9.385		1784	100 357 4
ANISOU		C	ALA			5.255	31.614	1.000 10.32
		0			1317	1335	1270	-181 99 5 4
ANISOU 2			ALA		10.266	6.134	31.701	1.000 10.97
			ALA		1389	1138	1641	-146 279 104
		N	THR		8.091	5.445	31.882	1.000 12.32
ANISOU			THR		1486	1547	1647	-314 563 -284
	2020		THR		7.626	6.715	32.421	1.000 12.28
ANISOU			THR		1717	1460	1489	-168 337 -200
	2021		THR		6.352	7.215	31.733	1.000 13.27
ANISOU 2			THR		2128	1182	1730	-258 -159 - 284
ATOM 2	2022	OG1	THR	293	5.317	6.237	31.911	1.000 13.85
ANISOU 2	2022	OG1	THR		1831	1217	2216	8 -131 7 4
	2023	CG2	THR		6.474	7.303	30.212	1.000 13.72
ANISOU 2	2023	CG2	THR		1791	1683	1738	-252 -56 -405
ATOM 2	2024	С	THR		7.363	6.635	33.937	1.000 10.58
ANISOU 2		С	THR		1439	1050	1533	12 447 9
	2025		THR		7.211	5.576	34.553	
ANISOU 2			THR		1049	1102		1.000 10.29
		Ň	PHE		7.243	7.810	1758	-56 93 1 1 8
ANISOU 2			PHE		1794		34.569	1.000 11.53
	2027		PHE			1093	1494	-307 306 - 66
ANISOU 2		CA		254	6.806	7.939	35.950	1.000 10.41
			PHE		1432	1061	1463	-174 125 -162
ANISOU 2		CB	PHE		6.709	9.426	36.336	1.000 12.25
			PHE		1930	1030	1694	-164 292 -64
	2029		PHE		6.270	9.658	37.770	1.000 12.77
ANISOU 2			PHE		1880	1136	1837	-103 178 -427
ATOM 2	2030	CDI	PHE		7.123	9.462	38.839	1.000 14.73
ANISOU 2	2030	CD1	PHE		1976	1893	1727	-539 161 -132
	2031			294	4.989	10.068	38.056	1.000 16.59
ANISOU 2				294	2180	1923	2199	348 386 -492
ATOM 2	2032	CE1	PHE	294	6.726	9.673	40.144	1.000 14.36
ANISOU 2	2032	CE1	PHE	294	1598	2028	1830	-505 280 -118
ATOM 2	2033	CE2	PHE		4.575	10.275	39.345	1.000 16.75
ANISOU 2	2033	CE2	PHE	294	2214	2062	2087	692 144 - 602
	2034		PHE		5.426	10.065	40.413	1.000 15.17
ANISOU 2			PHE		2040	1426	2296	
	2035		PHE		5.484	7.195	36.172	327 97 - 135
ANISOU 2	2035	Č	PHE		1401	1200	1536	1.000 10.89
	2036		PHE		5.325	6.425		-155 78 1 3 7
ANISOU 2			PHE		1396			1.000 10.67
	2037		GLN		4.487	1297	1360	90 337 1 0 5
ANISOU 2						7.355	35.299	1.000 10.62
	2037		GLN		1399	1187	1450	-18 88 - 24
ANISOU 2			GLN		3.217	6.612	35.393	1.000 11.31
			GLN		1433	1205	1660	-96 120 -321
	2039		GLN		2.284	7.053	34.254	1.000 11.66
ANISOU :			GLN		1425	1053	1953	-25 63 - 141
ATOM :	2040	CG	GLN		0.951	6.360	34.200	1.000 11.05
ANISOU :			GLN		1573	1011	1614	-93 -118 1 8
	2041		GLN	295	0.052	6.843	33.087	1.000 11.35
ANISOU:			GLN		1592	1326	1395	173 57 - 1 3
ATOM :	2042	OE1	GLN		0.349	7.823	32.378	1.000 15.06
ANISOU :	2042	OE1	GLN		2306	1589	1825	110 7 3 7 9
ATOM :	2043	NE2	GLN		-1.053	6.153	32.914	1.000 13.90
ANISOU :	2043	NE2	GLN		1511	1757	2015	156 -282 2 0 8
ATOM :	2044	C	GLN			5.107	35.389	1.000 10.12
					,	01	73.303	1.000 10.12

					- 157 -		
ANISOU			GLN	295 1154	1203	1486	21 160 -191
ATOM ANISOU	2045	0	GLN	295 2.82	4.309		1.000 37 82
ATOM	2045		GLN ASP	295 1264	1542	1686	-107 41 137
ANISOL	J 2046	5 N	ASP	296 4.26° 296 1076	4.558 1056	34.538	1.000 9.35
ATOM	2047	CA	ASP	296 4.655	3.172	1422 34.416	-118 -75 -275
ANISOU			ASP	296 1241	1139	1387	1.000 9 . 9 1 56 60 - 2 4 3
ATOM	2048	CB	ASP	296 5.699	2.852	33.347	1.000 10.26
ANISOU ATOM	2048		ASP	296 1315	1156	1429	113 132 - 36
ANISOU	2049	CG	ASP ASP	296 5.343 296 1357		31.885	1.000 11.42
ATOM	2050	OD1	ASP	296 4.143	1578 2.904	1405 31.531	358 121 -199
ANISOU	2050	OD1	ASP	296 1511	1744	1997	1.000 13.82 149 -209 - 62
ATOM	2051	OD2	ASP	296 6.282	3.151	31.047	1.000 13.48
ANISOU ATOM	2051			296 1802	1758	1564	228 364 7 3
ANISOU			ASP ASP	296 5.175 296 1416		35.770	1.000 10.31
ATOM	2053	0	ASP	296 4.852	1141 1.551	1361 36.197	16 91 - 198
ANISOU			ASP	296 1428	1452	1453	1.000 11.40 -288 32 3 5
ATOM	2054		TRP	297 6.004	3.484	36.441	1.000 10.88
ANISOU ATOM	2054		TRP	297 1752	1144	1238	-161 11 5 5
ANISOU	2055	CA	TRP TRP	297 6.646 297 1768		37.685	1.000 11.26
ATOM	2056		TRP	297 7.899	1215 3.999	1294	-217 -57 4 5
ANISOU	2056	CB	TRP	297 1387	1417	37.890 1112	1.000 10.31 -87 213 120
ATOM	2057	CG	TRP	297 8.621	3.651	39.172	-87 213 120 1.000 10.98
ANISOU ATOM	2057		TRP	297 1456	1394	1324	164 -29 -43
ANISOU	2058	CD2	TRP	297 9.082 297 1255			1.000 12.49
$\mathtt{ATOM}$	2059	CE2	TRP	297 9.692	1729 3.755	1761	75 - 298 - 197
ANISOU	2059	CE2	TRP	297 1860	2049	41.201 2202	1.000 16.08 -294 -977 4 9
ATOM	2060	CE3	TRP	297 9.040	5.910	40.379	1.000 17.41
ANISOU ATOM	2060	CE3	TRP	297 2778	1740	2096	-388 -916 - 234
ANISOU	2061	CDI	TRP	297 8.969 297 1617		39.589	1.000 13.58
ATOM	2062	NE1	TRP	297 9.614	1518 2.444	2025	0 -664 114
ANISOU	2062	NE1	TRP	297 2165	1909	40.808 2051	1.000 16.12 -22 -873 2 2 0
ATOM	2063	CZ2	TRP	297 10.24	3 4.320	42.341	1.000 19.85
ANISOU ATOM	2063	CZ2	TRP	297 2756	2383	2404	-951 -1337 267
ANISOU	2064	C23	TRP	297 9.586 297 4215		41.515	1.000 23.40
ATOM	2065	CH2	TRP	297 4215	2030	2645	-1001 -1757 - 77
ANISOU	2065	CH2	TRP	297 3178	2457	2537	1.000 21.51 -910 -1473 - 51
ATOM	2066	C	TRP	297 5.700	3.138	38.882	1.000 10.39
ANISOU ATOM	2066		TRP	297 1172	1448	1329	-280 -237 3 9 1
ANISOU			TRP TRP	297 5.574	2.159	39.639	1.000 13.52
ATOM	2068		ILE	297 1748 298 5.033	1830 4.272	1557	32 -91 7 0 3
ANISOU	2068	N	ILE	298 1400	1710	39.079 1480	1.000 12.08 -49 83 4 5 1
ATOM	2069	CA	ILE	298 4.223	4.521	40.272	1.000 13.43
ANISOU ATOM			ILE	298 1301	2484	1317	-199 -158 - 3 3
ANISOU	2070	CB	ILE	298 4.370	5.988	40.689	1.000 16.97
ATOM	2071	CG2	ILE	298 1877 298 3.538	2908 6.423	1661	-1000 214 -630
ANISOU	2071	CG2	ILE	298 3980	3121	41.876 1263	1.000 22.01 -233 546 -339
ATOM	2072	CG1	ILE	298 5.847	6.253	41.037	1.000 27.10
ANISOU ATOM	2072	CG1	ILE	298 2588	5151	2557	-2140 -708 9 7
ANISOU	2073		ILE	298 6.365	5.522	42.266	1.000 43.13
ATOM	2074		ILE	298 5185 298 2.772	8299 4.116	2904	-3717 -3055 7 0 8
ANISOU	2074	Č	ILE	298 1350	1652	40.131 1156	1.000 10.94 -165 -79 9 6
						~ <del>~ ~ ~ 0</del>	-165 -79 9 6

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						- 158 -		
ATOM	2075	0	ILE	298	2.137	3.844	41 155	1 000 12 67
ANISOU			ILE		1689			1.000 12.67
ATOM	2076					1634	1493	-102 212 352
			GLY		2.267	4.077	38.897	1.000 10.14
ANISOU			GLY		1412	1057	1384	-51 -377 2 0 1
MOTA	2077		GLY	299	0.866	3.822	38.695	1.000 10.72
ANISOU	2077	CA	GLY	299	1335	1084	1655	0 -229 -206
ATOM	2078	С	GLY		0.049	5.054		1.000 12.05
ANISOU		Č	GLY		1422	1293	1864	
ATOM	2079		GLY		0.585			
ANISOU		-				6.088	37.976	1.000 13.11
			GLY		1917	1199	1866	174 80 - 23
ATOM	2080		GLY		-1.268	4.931	38.490	1.000 13.92
ANISOU			GLY		1393	1531	2363	182 -410 - 223
ATOM	2081		GLY		-2.237	5.932	38.087	1.000 14.02
ANISOU	2081	CA	GLY	300	1524	1471		217 -563 - 336
ATOM	2082	С	GLY		-2.587	7.015		1.000 11.97
ANISOU			GLY		940 160			-488 -295
ATOM	2083		GLY		-3.322	7.950	38.722	
ANISOU			GLY		1219			1.000 10.90
ATOM	2084		ASN			1408	1515	-37 -203 - 134
					-2.090	6.910		1.000 11.64
ANISOU			ASN		948 155		17 -38	
ATOM	2085		ASN		-2.195	7.915		1.000 13.39
ANISOU		CA	ASN	30 <u>1</u>	1626	1904	1557	-191 -403 1 8 3
ATOM	2086	CB	ASN	301	-3.047	7.301	42.427	1.000 17.60
ANISOU	2086	CB	ASN	301	1391	2869	2426	-9 326 2 2 8
ATOM	2087	CG	ASN		-4.021	8 196	43.108	1.000 19.15
ANISOU			ASN		2549	2869 8.196 2827	1900	
ATOM		OD1			-5.072			805 59 3 7 7
ANISOU	2000		V C VI			8.606	42.591	1.000 15.47
					1258	2340	2280	-253 339 - 8
ATOM	2089	ND2	ASN		-3.661	8.510		1.000 29.28
ANISOU					3585	4783	2758	1521 -850 -885
ATOM	2090	С	ASN		-0.862	8.331	41.914	1.000 11.31
ANISOU			ASN	301	1436	1669	1194	1 1 -168
MOTA	2091	0	ASN	301	-0.033	7.456	42.221	1.000 12.03
ANISOU	2091	0	ASN		1483	1548	1542	-151 -279 8 2
ATOM	2092		TYR		-0.634	9.628	42.133	1.000 11.53
ANISOU			TYR		1186	1584	1611	
ATOM		CA	TYR		0.573			-61 26 1 0 2
ANISOU						10.046	42.838	1.000 11.90
		CA	TYR		1260	1395	1865	5 -212 225
ATOM	2094		TYR		0.657	11.589	43.036	1.000 13.14
ANISOU			TYR		1768	1404	1820	-273 190 181
MOTA	2095		TYR	302	1.082	12.287	41.750	1.000 10.88
ANISOU	2095	CG	TYR	302	1395	1347	1393	-321 2 -153
ATOM	2096	CD1			2.421	12.439	41.413	1.000 11.29
ANISOU					1385	1246	1659	-58 98 - 46
MOTA	2097				2.859	13.075		
ANISOU	2007	CEI	T I I				40.248	1.000 10.60
ATOM	2098				1055	1241	1732	-11 52 - 1
					0.161	12.793	40.858	1.000 11.30
ANISOU					1304	1332	1656	<b>-145</b> 105 - 26
MOTA	2099			302	0.573	13.406	39.690	1.000 11.72
ANISOU			TYR	302	1013	1733	1708	-288 -138 1 6 1
MOTA	2100	CZ	TYR	302	1.907	13.551	39.375	1.000 10.35
ANISOU			TYR		1009	1214	1709	-229 -50 -19
ATOM	2101		TYR	302				
ANISOU			TYR		1192	14.153	38.202	1.000 11.82
ATOM	2101					1532	1766	-8 102 1 0 4
			TYR		0.654	9.349	44.196	1.000 12.45
ANISOU		C	TYR		1517	1450	1765	-181 -202 2 1 7
ATOM	2103	0	TYR	302		9.230	44.878	1.000 13.55
ANISOU			TYR	302	1464	1925	1759	-339 -211 7
MOTA	2104	N	VAL	303	1.868	8.967	44.542	1.000 12.06
ANISOU			VAL		1517	1653	1413	-135 -3 3 4 0
ATOM	21.05		VAL		2.309	8.430	45.820	
-						J . Z J U	<del>-</del>	T.000 TT.00

			- 159 -		
	VAL 303	1434	1609	1471	-368 -197 2 2 3
		2.755	6.967		1.000 14.57
		1395	1682	2459	$-217 - 9\overline{18} \ 3 \ 1 \ 2$
ATOM 2107 CG1 ANISOU 2107 CG1		3.131 2644	6.462	47.132	1,000 1.7.33
ATOM 2108 CG2		1.703	1608 6.041	2331 45.122	-48 -1114 6 1 1.000 14.80
ANISOU 2108 CG2	VAL 303	1876	1676	2069	-592 -639 3 2 2
		3.467	9.328		1.000 13.88
		870 1791	261	L3 75	-286 - 375
		4.526	9.417		1.000 19.70
		1064 3.271	2307	4114	-61 323 -999
		1681	10.046 1815	47.393 1737	1.000 13.77 -479 -388 1 4 0
		4.205		47.828	1.000 13.37
	ASN 304	1626	1240	2212	-213 -533 2 7 9
			12.223		1.000 13.24
		1206		2370	-243 -344 2 9 6
		2.457 1142	12.922 2326	47.667 1910	1.000 14.16 146 -88 230
ATOM 2115 OD1			13.283	1910 46.540	146 -88 230 1.000 16.65
ANISOU 2115 OD1	ASN 304	1408	2456	2464	107 185 916
ATOM 2116 ND2		1.263		48.209	1.000 17.45
ANISOU 2116 ND2 ATOM 2117 C		1414 5.325	2961	2257	545 181 315
		1382	10.588 1299	48.728 1566	1.000 11.18 -183 -163 1 1 2
ATOM 2118 0				48.699	1.000 12.07
		1325	1382	1879	<b>-167 -66 -59</b>
		5.092	9.541	49.516	1.000 12.56
	ILE 305 ILE 305	1791 6.063	1296 9.011	1685 50.463	-152 -232 2 0 2 1.000 14.01
		2314	9.011 1393	1614	-55 -479 7 9
ATOM 2121 CB	ILE 305	5.781	9.493	51.906	1.000 14.44
		2223	1604	1659	-29 -217 1 5 7
ATOM 2122 CG2 : ANISOU 2122 CG2 :					1.000 15.31
ATOM 2123 CG1			1608 8.853	2441 52.498	43 -479 -314 1.000 14.83
ANISOU 2123 CG1		1779	1694	2163	27 -307 -153
ATOM 2124 CD1	ILE 305	4.163			1.000 28.68
ANISOU 2124 CD1		3788	9.252 5324	1786	-1491 381 9 2
		6.059 1703	7.487 1355	50.389	1.000 12.79
			6 864	1800	-260 -586 2 3 1 1.000 15.63
ANISOU 2126 O	ILE 305	1779	1564	2597	-185 -1008 2 7 7
		7.170	6.896	50.829	1.000 13.04
	ARG .306		1389	1946	-368 -598 3 8 3
		7.340 1352	5.435 1366	50.868 1773	1.000 11.82
		8.111	4.965	49.640	-375 -154 4 4 4 1.000 15.28
ANISOU 2129 CB		1976	1941	1886	-368 -19 111
ATOM 2130 CG		8.203	3.472	49.395	1.000 17.16
		2566	1953	2001	-68 -68 7 6
	ARG 306 ARG 306	8.344 2921	3.075 2361	47.937 2130	1.000 19.51
ATOM 2132 NE		7.078	3.198	47.212	-397 -396 - 302 1.000 20.65
ANISOU 2132 NE	ARG 306	2693	2844	2309	-1056 -310 2 1 4
		6.948	3.186	45.893	1.000 17.11
ANISOU 2133 CZ ATOM 2134 NH1		2006 8.013	2225	2268	45 -91 5 9 6
ANISOU 2134 NH1		2405	3.065 2677	45.083 3116	1.000 21.58 -232 381 -669
ATOM 2135 NH2	ARG 306	5.734	3.301	45.365	1.000 17.51
ANISOU 2135 NH2		2235	1550	2868	150 -484 - 162

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ATOM	2136	С	ARG	306	8.035	5.027	52.155	1 000 12 45
ANISOU	2136	С	ARG	306	2254	1018	1837	
ATOM	2137	0	ARG		9.006	5.682	52.556	-246 <u>-4</u> 81 9 8 1.000 12.15
ANISOU	2137	0	ARG		1902	1099	1615	
ATOM	2138	N	ARG		7.571	3.968	52.811	=18 -362 - 80 1.000 18.19
ANISOU	2138	N	ARG		3073	1620	2218	-734 -938 7 9 2
MOTA	2139		ARG		8.197	3.380	53.989	1.000 19.20
ANISOU	2139	CA	ARG		3053	1963	2277	-675 -1236 643
ATOM	2140	С	ARG		9.086	2.191	53.611	1.000 23.08
ANISOU			ARG	307	4018	1905	2847	-270 -1885 3 2 9
ATOM	2141		ARG		8.636	1.292	52.895	1.000 35.93
ANISOU			ARG		6003	2403	5244	38 -3227 - 791
ATOM	2142		ARG		7.131	2.918	54.997	1.000 28.25
ANISOU			ARG		5557	3297	1882	-1503 -277 5 0 9
ATOM	2143		ARG	307	6.032	3.921	55.275	1.000 33.39
ANISOU			ARG		4564	4859	3261	-1613 731 208
ATOM	2144	CD	ARG	307	5.022	3.523	56.317	1.000 40.42
ANISOU			ARG		6335	5701	3322	-1900 1263 9 7 1
ATOM	2145		ARG	307	5.605	2.952	57.529	1.000 50.83
ANISOU			ARG		8119	7287	3908	-2786 105 1624
ATOM	2146		ARG		4.894	2.441	58.530	1.000 51.36
ANISOU			ARG	307	7424	8064	4025	-3650 -966 2451
ATOM	2147	NHI	ARG	307	3.567	2.422	58.485	1.000 69.51
ANISOU	214/	NH1	ARG	307	7586	10951	7874	-6970 -2008 3 2 4 5
ATOM	2148	NH2	ARG		5.489	1.937	59.600	1.000 59.99
ANISOU	2148	NH2			10714	8150	3930	-5986 -3291 2028
ATOM	2149		THR		10.347	2.147	54.048	1.000 22.92
ANISOU			THR		2759	2587	3364	-589 -200 1 7 0
ATOM ANISOU	2150		THR		11.215	1.009	53.794	1.000 24.47
ATOM	2150		THR		3382	2649	3268	-360 52 1 5 0
ANISOU			THR	308	10.602	-0.252	54.382	1.000 31.10
ATOM	2151		THR		5251	2520	4044	-768 16 2 7 9
ANISOU			THR		10.610	-1.292	53.718	1.000 31.44
ATOM	2153		THR THR		4573	2676	4696	-457 -1745 - 40
ANISOU					12.615	1.279	54.378	1.000 23.51
ATOM	2154		THR		3718	2086	3131	413 -694 5 4 2
ANISOU	2154	001	THR THR		13.195	2.410	53.705	1.000 23.61
ATOM	2155				2711	2503	3754	153 437 - 9
ANISOU	2155	CG2	THR		13.573 4427	0.141	54.117	1.000 26.37
ATOM	2156		SER		10.066	2796	2796	927 -329 - 18
ANISOU	2156	N	SER		3759	-0.156	55.596	1.000 28.39
ATOM	2157		SER		9.488	2774 -1.335	4252	-19 2 1300
ANISOU	2157	CA	SER		6110		56.238	1.000 34.69
ATOM	2158		SER		8.109	3146 -1.737	3925	-1066 -1089 1626
ANISOU	2158	č	SER		6442	3910	55.724	
ATOM	2159		SER		7.672	-2.884	5383	-2171 -1170 2144
ANISOU	2159	Ō	SER		11389	5141	55.952	1.000 57.05
ATOM	2160		SER		9.450	-1.104	5146	-4907 -2077 2027
ANISOU	2160	CB	SER		4863	2958	57.755 4188	1.000 31.61
ATOM	2161		SER		8.485	-0.135	58.107	-483 368 962
ANISOU	2161	OG	SER		4731	3477	6604	1.000 38.99
MOTA	2162	N	LYS		7.391	-0.868	55.032	313 -2249 -496 1.000 47.69
ANISOU			LYS		5502	5577	7040	
ATOM	2163	FΕ	IUM		8.574	13.466	54.055	-539 -1369 1583 1.000 11.05
ANISOU		FΕ	IUM		1690	1156	1351	-101 -237 7 1
MOTA	2164		AKG		5.987	14.815	54.612	1.000 19.65
ANISOU	2164	C1	AKG	313	2777	2119	2572	258 -117 5 5 6
MOTA	2165		AKG		4.799	15.240	54.659	1.000 20.82
ANISOU			AKG		2957	2293	2659	514 -234 2 6 4
ATOM	2166	02	AKG		6.643	14.144	53.787	1.000 17.79
						~		2.000 17.75

- 161 -ANISOU 2166 02 AKG 313 2407 1765 2587 74 - 377 429 2167 C2 MOTA AKG 313 6.867 15.178 55.844 1.000 20,08 ANISOU 2167 C2 313 1997 313 7.982 AKG 2566 3068 -528 419 -399 2168 05 ATOM AKG 14.661 55.821 1.000 17.60 313 2289 ANISOU 2168 O5 AKG 2066 2334 -314 226 -252 ATOM 2169 C3 AKG 313 6.272 16.080 56.872 1.000 21.69 ANISOU 2169 C3 AKG 313 2751 1910 3581 240 62 - 327 16.741 57.716 1.000 21.50 313 7.318 2170 C4 ATOM AKG ANISOU 2170 C4 313 3246 AKG 1761 3160 199 -143 - 185 17.816 58.672 1.000 22.58 MOTA 2171 C5 AKG 313 6.923 ANISOU 2171 C5 AKG 313 3122 1840 3618 755 -495 - 313 2172 03 MOTA 18.591 59.124 1.000 27.48 AKG 313 7.754 ANISOU 2172 03 AKG 313 3581 2470 4389 -34 602 -1266 ATOM 2173 04 AKG 313 5.660 17.889 58.999 1.000 28.55 ANISOU 2173 04 AKG 313 3191 2809 4846 612 -246 -1148 2174 S ATOM SO4 401 11.676 0.439 24.942 1.000 40.14 2175 O1 2176 O2 ATOM SO4 401 11.293 0.826 26.321 1.000 33.12 MOTA SO4 401 12.501 -0.829 25.014 1.000 35.79 2177 03 MOTA SO4 401 10.430 0.189 24.129 1.000 54.89 2178 04 401 12.500 1.520 MOTA SO4 24.329 1.000 44.80 2179 OW MOTA HOH 501 -6.455 10.219 44.319 1.000 14.29 MOTA 2180 OW 502 -10.520 18.612 50.560 1.000 12.86 HOH 2181 OW MOTA HOH 503 -8.644 16.907 47.858 1.000 16.83 MOTA 2182 OW HOH 504 -10.313 20.800 43.074 1.000 16.10 52.602 1.000 16.38 47.100 1.000 20.55 46.406 1.000 27.41 MOTA 2183 OW HOH 505 -6.051 19.199 ATOM 2184 OW HOH 506 -6.873 24.642 MOTA 2185 OW 507 10.676 -4.179 HOH MOTA 2186 OW HOH 508 -0.077 21.786 40.872 1.000 15.22 MOTA 2187 OW HOH 509 5.761 46.041 1.000 17.40 13.656 MOTA 2188 OW HOH 510 29.135 31.449 51.982 1.000 18.40 2189 OW MOTA HOH 511 26.032 32.724 52.741 1.000 17.03 2190 OW MOTA HOH 512 10.965 32.371 46.000 1.000 16.70 MOTA 2191 OW HOH 513 23.871 58.649 1.000 18.71 24.457 2192 OW MOTA нон 514 26.353 29.063 50.326 1.000 18.96 MOTA 2193 OW нон 515 23.191 33.106 53.153 1.000 20.41 MOTA 2194 OW HOH 516 21.429 11.721 55.329 1.000 18.39 MOTA 2195 OW 517 9.122 HOH 15.567 53.585 1.000 24.87 MOTA 2196 OW HOH 518 27.843 17.352 53.437 1.000 27.76 2197 OW MOTA 519 -14.415 20.029 44.444 1.000 23.47 HOH 2198 OW MOTA HOH 520 15.253 33.050 51.771 1.000 27.20 MOTA 2199 OW HOH 521 14.080 31.486 44.302 1.000 21.58 522 17.770 523 3.671 2200 OW MOTA HOH 33.842 53.596 1.000 23.56 MOTA 2201 OW HOH 24.673 36.173 1.000 20.95 MOTA 2202 OW 524 -15.683 28.618 525 -5.386 20.413 HOH 52.535 1.000 24.05 MOTA 2203 OW HOH 39.013 1.000 26.85 58.778 62.202 55.737 MOTA 2204 OW нон 526 10.417 27.949 1.000 28.33 527 23.165 1.000 29.36 ATOM 2205 OW HOH 19.592 ATOM 2206 OW 528 23.736 HOH 10.550 1.000 24.02 MOTA 2207 OW HOH 529 -1.662 28.650 42.485 1.000 21.62 MOTA 2208 OW 530 -4.689 10.177 46.511 HOH 1.000 31.65 MOTA 2209 OW 531 1.545 HOH 35.657 50.866 1.000 19.59 2210 OW MOTA HOH 532 0.980 36.818 1.000 30.57 22.687 2211 OW ATOM HOH 533 -12.450 16.848 56.071 1.000 28.42 ATOM 2212 OW HOH 534 -9.418 16.139 51.364 1.000 22.60 2213 OW ATOM HOH 535 32.711 25.816 43.116 1.000 31.44 2214 OW MOTA HOH 536 27.068 24.587 55.468 1.000 23.32 2215 OW ATOM HOH 537 13.523 11.832 51.199 1.000 10.73 MOTA 2216 OW нон 538 8.513 16.158 35.074 1.000 12.26 MOTA 2217 OW нон 539 0.922 35.058 1.000 14.79 2.590 MOTA 2218 OW HOH 540 -1.548 34.484 1.000 14.25 3.709 MOTA 2219 OW HOH 541 11.711 16.898 30.416 1.000 17.84

- 162 -ATOM 2220 OW нон 542 15.389 11.536 32.065 1.000 17.88 ATOM 2221 OW нон 543 18.496 6.995 52.191 1.000 1-7-247 ATOM 2222 OW HOH 544 19.848 22.580 35.334 1.000 17.28 ATOM 2223 OW HOH 545 -0.387 4.787 41.967 1:000 13.22 MOTA 2224 OW 546 23.502 нон 12.662 35.308 1.000 18.14 2225 OW ATOM HOH 547 10.332 25.236 33.926 1.000 19.05 ATOM 2226 OW HOH 548 21.447 20.605 34.090 1.000 17.24 ATOM 2227 OW HOH 549 8.164 7.685 27.077 1.000 25.40 ATOM 2228 OW HOH 550 14.393 -5.127 40.321 1.000 15.88 2229 OW ATOM HOH 551 12.873 29.356 39.662 1.000 16.45 MOTA 2230 OW НОН 552 11.974 58.426 1.000 19.71 33.182 1.000 17.90 43.340 1.000 23.76 40.079 1.000 18.44 24.144 ATOM 2231 OW нон 553 17.521 7.949 MOTA 2232 OW нон 554 3.401 2.691 MOTA 2233 OW HOH 555 18.669 28.057 ATOM 2234 OW НОН 556 10.827 12.928 30.017 1.000 19.57 ATOM 2235 OW нон 557 20.630 66.466 1.000 20.84 64.044 1.000 21.62 16.270 ATOM 2236 OW HOH 558 11.315 20.266 ATOM 2237 OW нон 559 26.277 14.516 43.946 1.000 16.22 2238 OW ATOM нон 560 9.616 15.488 32.365 1.000 19.40 2239 OW ATOM нон 561 8.888  $27.857 \ 1.000 \ \overline{22.74}$ 4.903 MOTA 2240 OW нон 562 20.496 -1.851 42.511 1.000 22.98 ATOM 2241 OW HOH 563 17.033 29.415 38.332 1.000 26.36 ATOM 2242 OW HOH 564 18.595 6.141 37.697 1.000 25.10 565 22.446 566 6.586 567 6.250 568 7.341 569 16.090 ATOM 2243 OW HOH 13.893 31.420 1.000 29.00 ATOM 2244 OW HOH 3.577 28.350 1.000 27.82 ATOM 2245 OW HOH 20.077 30.961 1.000 23.27 MOTA 2246 OW HOH 16.113 31.186 1.000 28.59 ATOM 2247 OW HOH 32.070 42.552 1.000 33.08 ATOM 2248 OW HOH 570 11.500 28.806 37.258 1.000 25.17 2249 OW ATOM HOH 571 12.901 26.768 58.591 1.000 28.58 572 -17.071 17.043 50.450 1.000 28.82 573 25.262 7.705 37.199 1.000 39.05 571 12.901 ATOM 2250 OW HOH ATOM 2251 OW HOH 37.199 1.000 39.05 ATOM 2252 OW HOH 574 32.884 26.440 51.734 1.000 29.03 ATOM 2253 OW 575 -1.199 HOH 19.088 42.527 1.000 14.86 ATOM 2254 OW HOH 576 -4.389 33.026 25.732 63.392 1.000 29.56 ATOM 2255 OW нон 577 17.569 32.249 1.000 20.62 ATOM 2256 OW нон 578 -19.107 12.822 67.516 1.000 22.35 ATOM 2257 OW нон 579 29.333 19.198 51.975 1.000 22.51 ATOM 2258 OW 580 27.950 HOH 51.903 1.000 25.40 68.535 1.000 21.19 33.953 1.000 25.29 27.635 ATOM 2259 OW НОН 581 -21.085 14.501 MOTA 2260 OW HOH 582 1.529 17.378 17.378 33.953 1.000 25.29 20.887 66.894 1.000 33.92 5 19.091 44.780 1.000 17.48 12.597 43.347 1.000 22.09 21.268 29.046 1.000 20.79 0 25.438 41.729 1.000 29.68 1.046 29.689 1.000 27.70 13.540 42.235 1.000 25.91 14.852 34.021 1.000 26.77 ATOM 2261 OW НОН 583 9.138 ATOM 2262 OW 584 -11.896 19.091 HOH ATOM 2263 OW HOH 585 6.382 ATOM 2264 OW HOH 586 17.762 21.268 ATOM 2265 OW 587 -11.500 25.438 HOH MOTA 2266 OW нон 588 7.877 MOTA 2267 OW НОН 589 27.985 ATOM 2268 OW HOH 590 1.276 MOTA 2269 OW 41.242 1.000 26.77 36.006 1.000 27.92 57.827 1.000 31.86 39.940 1.000 32.07 HOH 591 24.622 24.179 MOTA 2270 OW HOH 592 0.404 14.096 MOTA 2271 OW HOH 593 -2.835 36.981 57.827 MOTA 2272 OW HOH 594 3.276 0.788 ATOM 2273 OW НОН 595 11.025 -8.794 31.468 1.000 27.18 2274 OW ATOM HOH 596 6.301 2.276 42.639 1.000 29.74 2275 OW ATOM HOH 597 29.302 62.924 16.146 1.000 43.75 ATOM 2276. OW нон 598 19.039 20.964 67.011 1.000 30.85 ATOM 2277 OW 599 8.380 HOH 22.088 64.518 1.000 42.62 2278 OW ATOM HOH 600 21.480 10.826 34.742 1.000 25.74 2279 OW ATOM HOH 601 -2.907 21.956 38.566 1.000 30.92 2280 OW ATOM HOH 602 -3.928 29.841 43.352 1.000 43.96

- 163 -2281 OW MOTA нон 603 2.885 21.563 34.437 1.000 33.10 MOTA 2282 OW HOH 604 11.801 6.043 25.270 1.000 3-8,18 6.043 25.270 1.000 ± a.10 17.197 40.472 1.000 18.48 23.349 68.110 1.000 22.54 ATOM 2283 OW HOH 605 -1.019 ATOM 2284 OW HOH 606 18.382 2285 OW ATOM HOH 607 -8.141 8.137 45.609 1.000 17.64 MOTA 2286 OW нон 608 5.022 51.700 1.000 24.29 2.667 ATOM 2287 OW 10.755 33.490 1.000 21.94 HOH 609 17.557 MOTA 2288 OW нон 610 11.222 1.201 49.675 1.000 20.61 2289 OW 611 4.243 MOTA HOH 35.047 50.509 1.000 22.18 2290 OW MOTA HOH 612 11.103 56.082 1.000 22.08 4.031 ATOM 2291 OW 613 11.366 31.522 36.791 1.000 32.32 нон 2292 OW MOTA HOH 614 -21.189 24.787 52.739 1.000 31.83 MOTA 2293 OW нон 615 7.847 -1.491 30.674 1.000 24.77 2294 OW 616 19.041 11.937 31.445 1.000 25.97 MOTA нон MOTA 2295 OW 617 6.221 нон 29.879 40.410 1.000 29.24 618 17.266 5.933 ATOM 2296 OW HOH 35.280 1.000 23.72 2297 OW ATOM HOH 619 5.983 -7.215 28.510 1.000 28.19 620 22.574 8.129 57.639 1.000 30.97 621 2.553 7.806 60.287 1.000 28.77 2298 OW MOTA HOH MOTA 2299 OW нон 25.812 51.234 1.000 34.00 34.823 53.632 1.000 25.88 13.838 67.343 1.000 28.46 2300 OW MOTA нон 622 29.939 ATOM 2301 OW HOH 623 2.205 624 18.091 ATOM 2302 OW HOH 625 8.342 3.195 58.475 1.000 26.84 626 -16.086 18.427 42.790 1.000 31.11 627 -2.098 13.445 35.620 1.000 27.48 ATOM 2303 OW HOH ATOM 2304 OW нон MOTA 2305 OW HOH ATOM 2306 OW нон 628 0.481 30.471 42.834 1.000 32.55 ATOM 2307 OW HOH 629 13.368 33.845 42.899 1.000 28.70 ATOM 2308 OW 630 -13.792 14.642 51.533 1.000 25.58 HOH 2309 OW ATOM HOH 631 3.299 1.461 29.242 1.000 39.62 MOTA 2310 OW 632 -16.012 20.690 46.705 1.000 27.75 HOH 2311 OW MOTA нон 633 19.606 8.142 31.259 1.000 27.02 MOTA 2312 OW HOH 634 5.077 7.954 57.205 1.000 30.59 2313 OW MOTA 635 -1.502 6.963 нон 45.877 1.000 35.68 MOTA 2314 OW HOH 636 9.974 17.449 38.804 1.000 21.84 ATOM 2315 OW HOH 637 -22.829 12.836 67.228 1.000 25.04 MOTA 2316 OW нон 638 6.275 34.333 39.722 1.000 25.88 MOTA 2317 639 2.248 OW HOH 19.798 56.051 1.000 26.67 ATOM 2318 OW HOH 640 -20.552 17.013 67.454 1.000 31.34 MOTA 2319 OW 641 9.298 HOH 16.570 28.911 1.000 29.96 MOTA 2320 OW 642 -1.732 11.113 60.074 1.000 28.13 23.604 44.657 1.000 36.36 HOH MOTA 2321 OW 643 34.157 нон MOTA 2322 OW 644 24.298 33.576 1.000 34.90 31.570 1.000 32.66 20.199 нон MOTA 2323 OW нон 645 13.803 -4.667 MOTA 2324 OW 646 6.295 -2.594 29.009 1.000 34.61 49.318 1.000 28.08 HOH 2325 OW MOTA нон 647 5.623 37.039 MOTA 2326 OW 648 -18.805 19.286 46.868 1.000 38.32 HOH MOTA 2327 OW 649 16.026 35.829 49.382 1.000 34.45 650 -12.187 28.769 45.330 1.000 27.36 нон 649 16.026 35.829 ATOM 2328 OW HOH 2329 OW MOTA 55.101 1.000 27.43 нон 651 21.344 5.778 MOTA 2330 OW нон 652 -1.848 2.125 32.240 1.000 32.02 MOTA 2331 OW 653 -14.568 18.811 HOH 55.775 1.000 29.95 MOTA 2332 OW нон 654 -8.655 26.254 38.301 1.000 32.07 2333 OW MOTA нон 655 18.836 13.542 28.102 1.000 32.24 ATOM 2334 OW нон 656 16.217 14.669 25.619 1.000 33.35 MOTA 2335 OW 657 28.678 14.477 нон 38.043 1.000 30.94 MOTA 2336 OW нон 658 -11.834 15.408 53.330 1.000 33.25 ATOM 2337 OW HOH 659 -1.317 38.273 59.599 1.000 34.45 MOTA 660 8.784 2338 OW нон 13.918 28.681 1.000 33.62 MOTA 2339 OW HOH 661 -3.058 14.508 47.405 1.000 28.79 MOTA 2340 OW HOH 662 10.968 33.651 38.533 1.000 36.21 MOTA 2341 OW нон 663 28.960 21.602 53.665 1.000 29.25

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ATOM	2342	OW	нон	664	-10.709	26.808	39.175	1.000 42.71
ATOM	2343	OW	нон	665		7.093	55.023	
ATOM	2344	OW	нон	666	6.404	24.865	29.848	1.000 3-029
$\mathtt{ATOM}$	2345	OW	нон		-15.418	19.777	58.341	1.000 34.55
ATOM	2346	OW	нон	668		0.000	37.259	1000 33 .82
$\mathtt{MOTA}$	2347	OW	нон	669	19.652	24.610	33.660	0.330 49.90
ATOM	2348	OM	нон	670		9.619	29.950	1.000 31.77
$\mathtt{ATOM}$	2349	OW	HOH	671		2.958	28.338	1.000 29 . 94
ATOM	2350	OW	HOH	672	-0.059	3.652	30.079	1.000 34.94
ATOM	2351	OW	нон	673	29.037	20.923	56.153	1.000 32.23
ATOM	2352	ow	нон	674	-15.435	31.088	53.795	1.000 28.52
MOTA	2353	OM	нон		-12.846	21.220	61.856	1.000 38.79
ATOM	2354	OM	нон	676		39.666	49.554	1.000 40 . 30
ATOM	2355	OW	нон	677		28.822	41.521	1.000 34.01
ATOM	2356	OW	HOH	678	6.029	39.991	46.094	1.000 42.69
ATOM	2357	OW	нон	679	35.052	23.156	52.356	1.000 40.17
ATOM	2358	OW	HOH		-12.008	38.355	51.601	1.000 35.18
ATOM	2359	OW	HOH	681	3.061	13.047	53.152	1.000 35.17
ATOM	2360	OW	нон	682	1.379	2.075	27.532	1.000 46.38
ATOM	2361	OW	нон	683	-0.516	-2.480	37.686	1.000 21.77
ATOM	2362	OW	HOH	684	4.567	10.310	43.503	1.000 24.86
ATOM	2363	OW	нон	685	19.443	5.558	61.133	1.000 36.06
ATOM		OW	нон	686	3.205	29.499	40.656	1.000 36.99
ATOM	2365	OW	нон	687	32.498	16.774	43.447	1.000 41.18
ATOM	2366	OW	нон	688	28.166	23.113	57.593	1.000 35.56
ATOM		OW	нон	689	-17.023	23.220	46.759	1.000 30.05
ATOM	2368	OW	HOH	690	15.567	7.782	28.910	1.000 32.51
ATOM		OW	нон	691	11.780	30.287	57.203	1.000 33.34
MOTA		OW	нон	692	24.449	12.699	32.400	1.000 34.99
ATOM	2371	OW	нон	693	26.200	25.005	57.918	1.000 39.38
								000 37.38

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## **CLAIMS**

- Deacetoxycephalosporin C synthase (DAOCS) having a structure designated by the X-ray co-ordinates of structure A or structure B herein.
- 2. DAOCS in the form of a complex with a metal, e.g. iron or lead, and optionally in the presence of a substrate and/or a substrate analogue or inhibitor, having a structure designated by the X-ray co-ordinates herein.
- 3. DAOCS as claimed in claim 2, wherein the substrate is penicillin N, penicillin G, 2-oxoglutarate or dioxygen, and the inhibitor is selected from N-oxalylamino acids, pyridine-carboxylates and nitrous oxide.
- Use of the three-dimensional structure of DAOCS for the
   modification of DAOCS or other related 2-oxoglutarate dependent enzyme.
  - 5. Use as claimed in claim 4, wherein the related 2-oxoglutarate dependent enzyme is DACS, DAOC/DACS or the oxygenase enzyme involved in the introduction of the  $7\alpha$ -methoxy group into cephamycin C.
  - 6. Use as claimed in claim 5 for the modification of DAOCS, DACS or DAOC/DACS such that they accept unnatural substrates more efficiently than the wild type enzymes.

7. Use as claimed in claim 5 for the modification of DAOCS, DACS, DAOC/DACS such that they convert natural substrates to pharmaceuticals or useful intermediates in the preparation of pharmaceuticals.

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8. Use as claimed in claim 6 wherein the unnatural substrates are penicillins including penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, or penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain.

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- 9. Use as claimed in claim 6 wherein the unnatural substrate is a cephalosporin.
- 10. Use as claimed in claim 6 wherein the unnatural substrate is an amino acid, including the proteinogenic amino acids, or a peptide.
  - 11. Use as claimed in any one of claims 6-8, wherein penicillin G, penicillin V, another unnatural substrate or penicillin N is converted to a cephalosporin or exomethylene cephalosporin.

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An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be

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changed in order to accommodate the change in one of the above.

13. An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

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- 14. An enzyme according to claim 12 or claim 13 which is a mutant of DAOCS or DACS or DAOC/DACS.
- 15. An enzyme as claimed in any one of claims 12-14, wherein both the side chain and the penicillin/cephalosporin binding sites of penicillin N or DAOC are modified and at least one of the residues specified in claims 12 and 13 is changed or deleted.
- 16. An enzyme as claimed in any one of claims 12-15, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
  - 17. A gene encoding for the enzyme of any one of claims 12-16.

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- 18. A micro-organism capable of expressing the gene of claim 17 under fermentation conditions.
- 19. Use of micro-organisms of claim 18 for the production of
   30 beta-lactams of the penicillin or cephalosporin (including cepham) families.

- 20. Use as claimed in claim 19 wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway including isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
  - 21. A method which comprises using the three-dimensional structure of DAOCS for determining or predicting the structure of another related 2-oxoglutarate dependent enzyme or related enzyme not from the penicillin and cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the other enzyme or for designing an inhibitor for the other enzyme.
  - 22. A method as claimed in claim 21 wherein the said other related 2-oxoglutarate dependent enzyme or related enzyme is 1-aminocylopropane-1-carboxylate oxidase, gibberellin C-20 oxidase, flavone synthase, flavanone 3β-hydroxylase, hyoscyamine 6β-hydroxylase, prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, lysyl hydroxylase, proline hydroxylases, γ-butyrobetaine hydroxylase, enzymes in herbicide resistance mechanisms, clavaminate synthase, an oxygenase enzyme involved in the biosynthesis of carbapenems, the so called ethylene forming enzyme from *Pseudomonas syringe*, p-hydroxyphenylpyruvate dioxygenase, and an oxygenase enzyme involved in the oxidation of phytol in human liver peroxisomes.

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23. A method as claimed in claim 21 or 22, wherein the said other enzyme is modified, by deletion or addition or alteration; at one or more of the sites defined in claim 12 or claim 13; or using the following information for the design or an inhibitor: Asp185, His183 and His243 act as ligands to the iron; Arg258 and Ser260 and the Fe bind the

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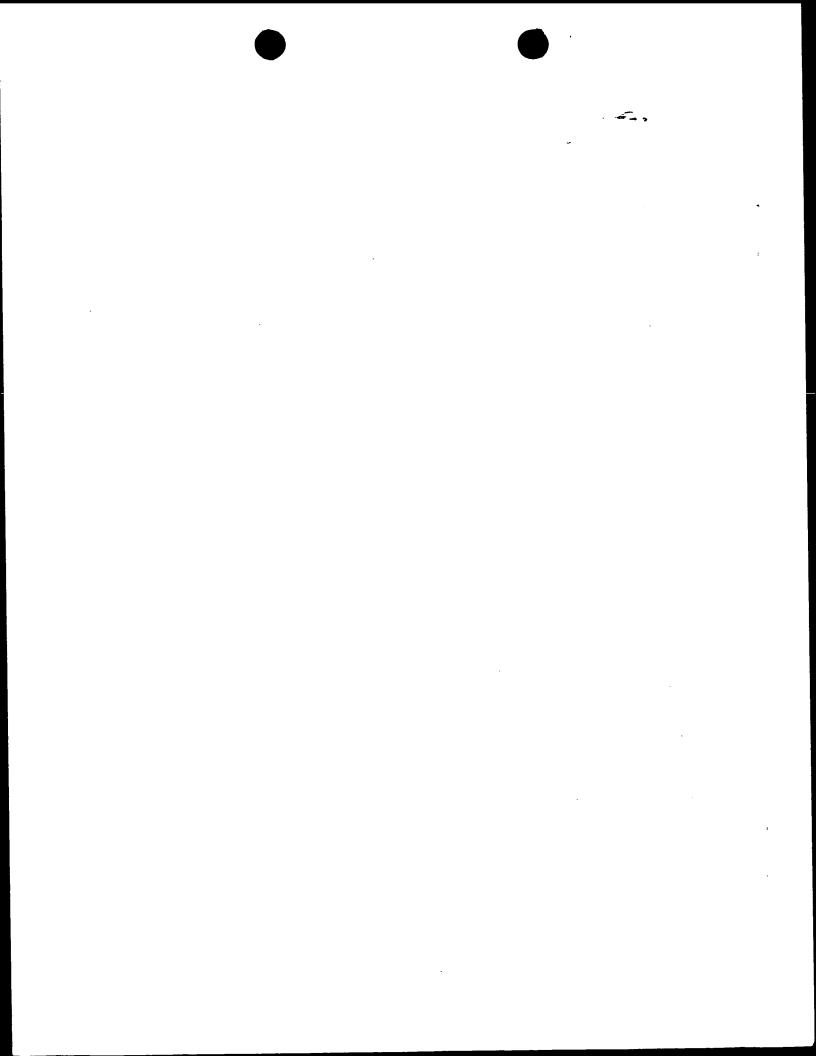
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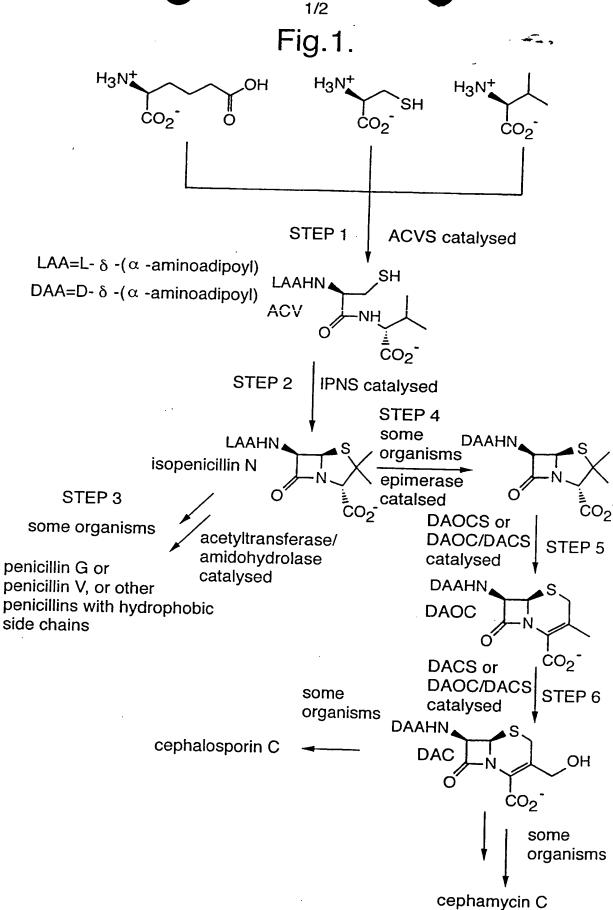
2-oxoglutarate; Met180, Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the construction of the part of the active site binding 2-oxoglutarate; and Arg160 and Arg162 are important for binding an amino acid or peptide derived substrate.

- A method as claimed in any one of claims 21-23, wherein the said other enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.
- 25. A method as claimed in any one of claims 21-23, wherein the said other enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.
- A method as claimed in any one of claims 21-23, wherein the said other enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.



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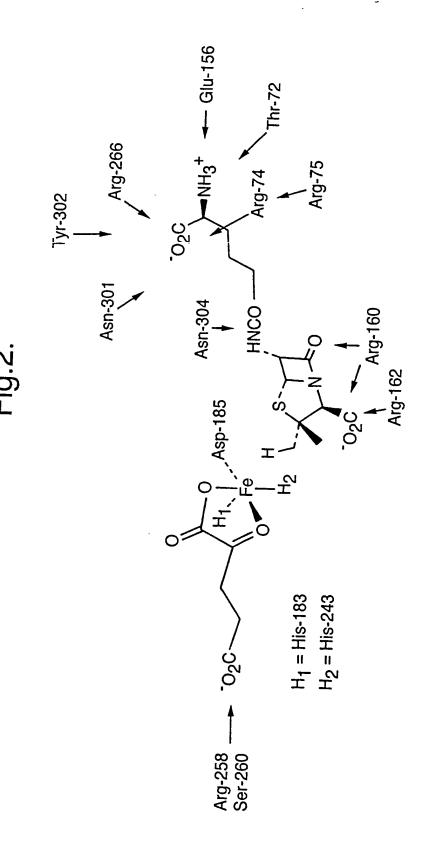
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SUBSTITUTE SHEET (RULE 26)

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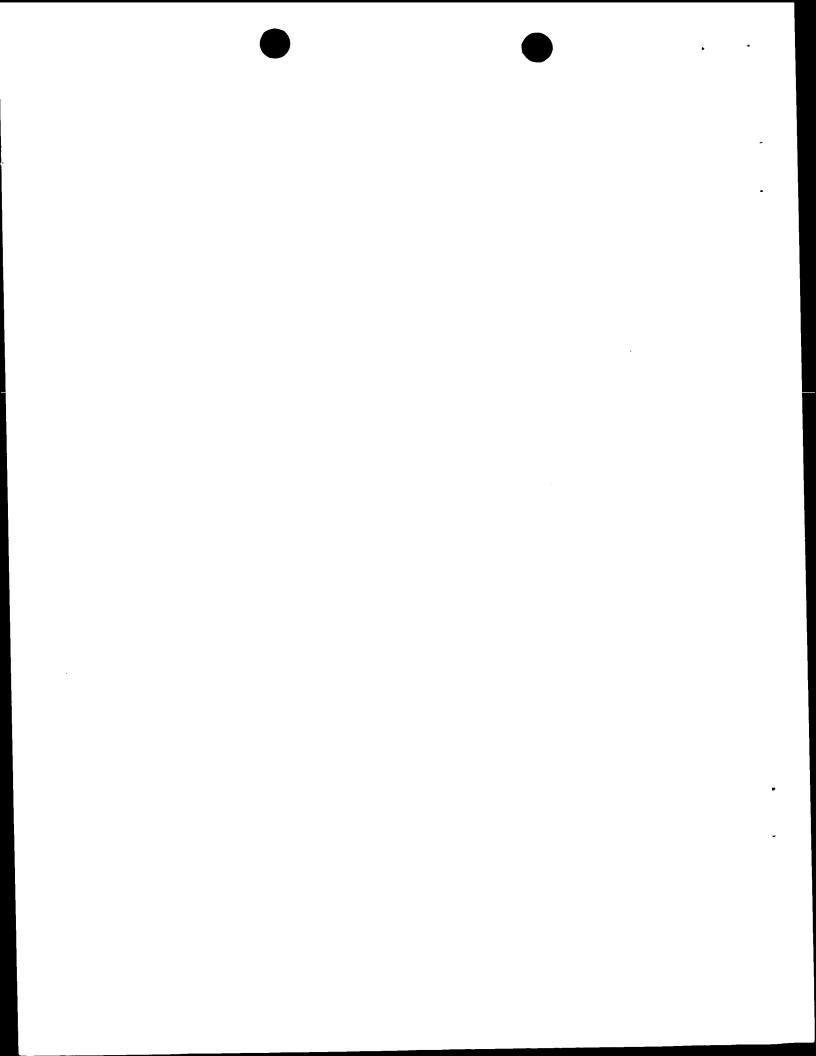
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## **CLAIMS**

- Deacetoxycephalosporin C synthase (DAOCS) having a structure designated by the X-ray co-ordinates of structure A or structure B herein.
- 2. DAOCS in the form of a complex with a metal, e.g. iron or lead, and optionally in the presence of a substrate and/or a substrate analogue or inhibitor, having a structure designated by the X-ray co-ordinates herein.
- 3. DAOCS as claimed in claim 2, wherein the substrate is penicillin N, penicillin G, 2-oxoglutarate or dioxygen, and the inhibitor is selected from N-oxalylamino acids, pyridine-carboxylates and nitrous oxide.
- Use of the three-dimensional structure of DAOCS for the
   modification of DAOCS or other related 2-oxoglutarate dependent enzyme.
  - 5. Use as claimed in claim 4, wherein the related 2-oxoglutarate dependent enzyme is DACS, DAOC/DACS or the oxygenase enzyme involved in the introduction of the  $7\alpha$ -methoxy group into cephamycin  $\acute{C}$ .
  - 6. Use as claimed in claim 5 for the modification of DAOCS, DACS or DAOC/DACS such that they accept unnatural substrates more efficiently than the wild type enzymes.



7. Use as claimed in claim 5 for the modification of DAOCS, DACS, DAOC/DACS such that they convert natural substrates to pharmaceuticals or useful intermediates in the preparation of pharmaceuticals.

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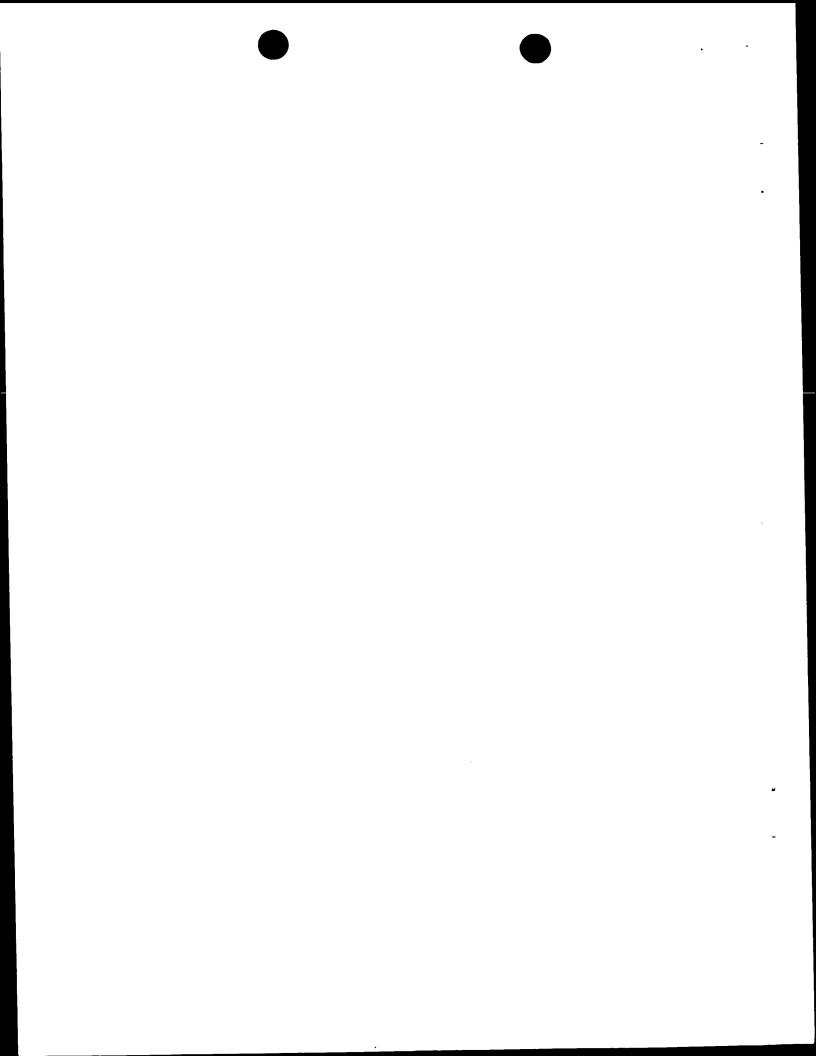
8. Use as claimed in claim 6 wherein the unnatural substrates are penicillins including penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, or penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain.

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- 9. Use as claimed in claim 6 wherein the unnatural substrate is a cephalosporin.
- 10. Use as claimed in claim 6 wherein the unnatural substrate is an amino acid, including the proteinogenic amino acids, or a peptide.
  - 11. Use as claimed in any one of claims 6-8, wherein penicillin G, penicillin V, another unnatural substrate or penicillin N is converted to a cephalosporin or exomethylene cephalosporin.

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- An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187,
- Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.



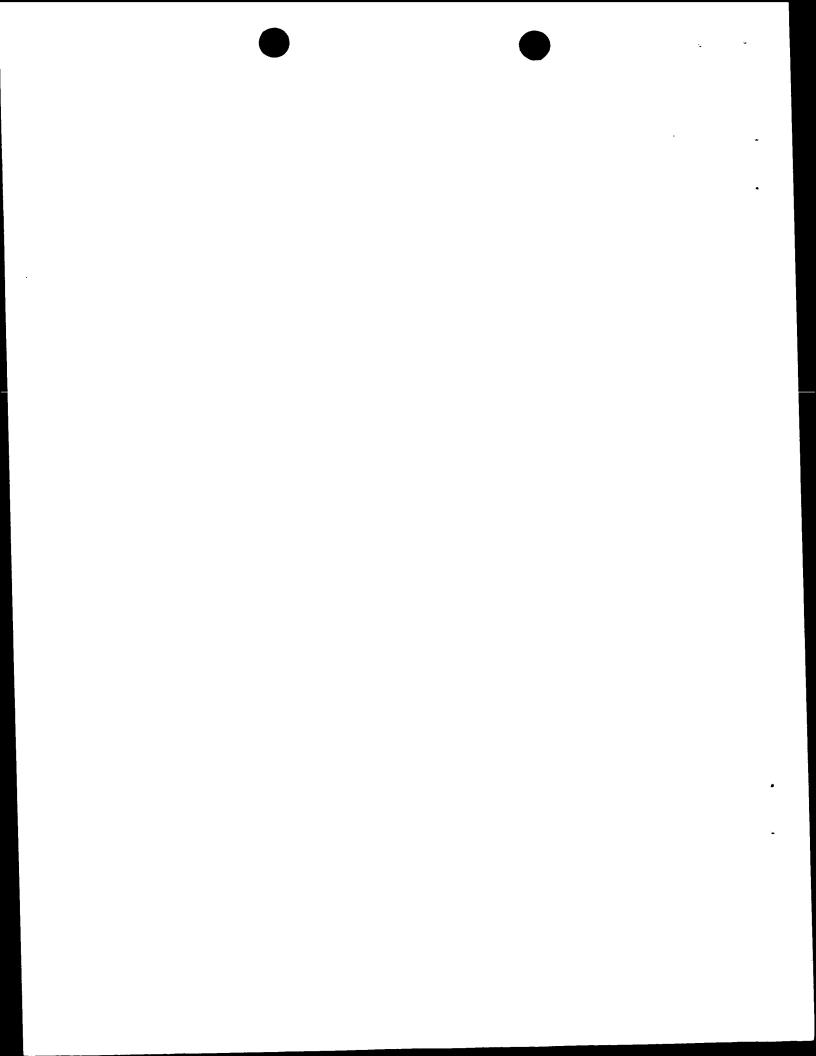
An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

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- 14. An enzyme according to claim 12 or claim 13 which is a mutant of DAOCS or DACS or DAOC/DACS.
- 15. An enzyme as claimed in any one of claims 12-14, wherein both the side chain and the penicillin/cephalosporin binding sites of penicillin N or DAOC are modified and at least one of the residues specified in claims 12 and 13 is changed or deleted.
- 16. An enzyme as claimed in any one of claims 12-15, wherein
  two or more complementary mutations are introduced to create or delete a
  binding interaction, including H-bonds, electrostatic, or hydrophobic
  interactions.
  - A gene encoding for the enzyme of any one of claims 12-16.

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- 18. A micro-organism capable of expressing the gene of claim 17 under fermentation conditions.
- 19. Use of micro-organisms of claim 18 for the production of
   30 beta-lactams of the penicillin or cephalosporin (including cepham) families.



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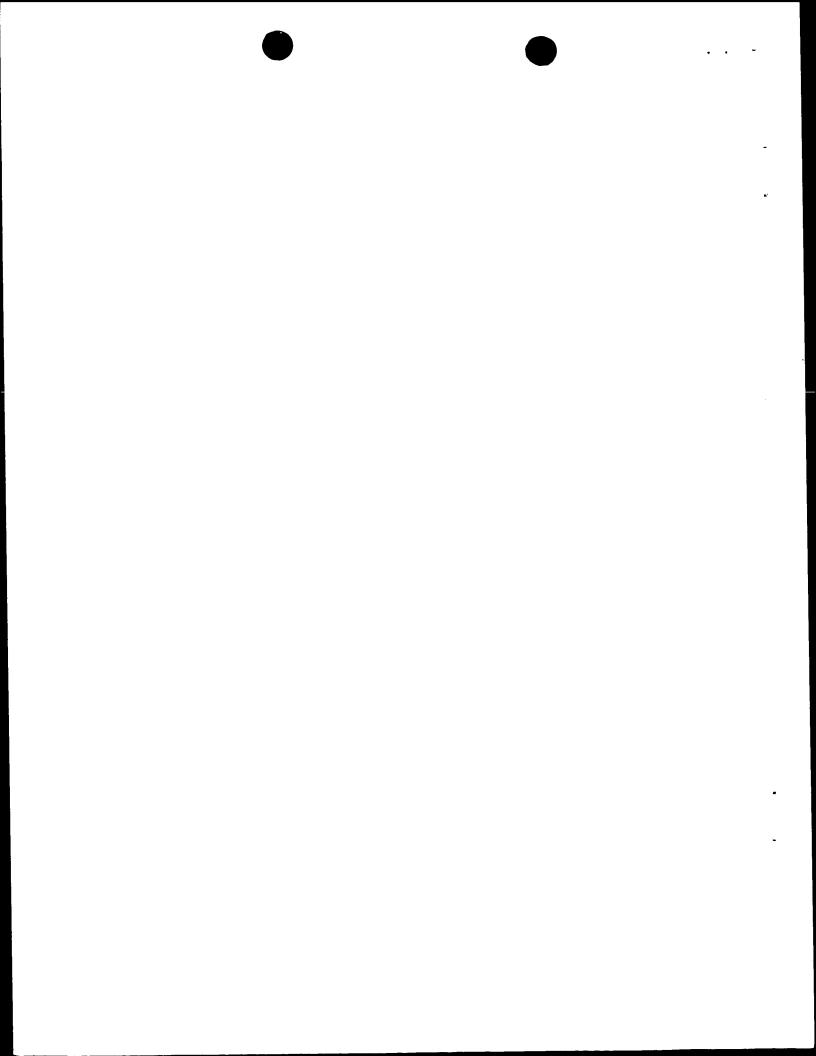
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- 20. Use as claimed in claim 19 wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway including isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 21. A method which comprises using the three-dimensional structure of DAOCS for determining or predicting the structure of another related 2-oxoglutarate dependent enzyme or related enzyme not from the penicillin and cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the other enzyme or for designing an inhibitor for the other enzyme.
- 22. A method as claimed in claim 21 wherein the said other related 2-oxoglutarate dependent enzyme or related enzyme is 1-aminocylopropane-1-carboxylate oxidase, gibberellin C-20 oxidase, flavone synthase, flavanone 3β-hydroxylase, hyoscyamine 6β-hydroxylase, prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, lysyl hydroxylase, proline hydroxylases, γ-butyrobetaine hydroxylase, enzymes in herbicide resistance mechanisms, clavaminate synthase, an oxygenase enzyme involved in the biosynthesis of carbapenems, the so called ethylene forming enzyme from *Pseudomonas syringe*, p-hydroxyphenylpyruvate dioxygenase, and an oxygenase enzyme involved in the oxidation of phytol in human liver peroxisomes.

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A method as claimed in claim 21 or 22, wherein the said other enzyme is modified, by deletion or addition or alteration; at one or more of the sites defined in claim 12 or claim 13; or using the following information for the design or an inhibitor: Asp185, His183 and His243 act as ligands to the iron; Arg258 and Ser260 and the Fe bind the



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2-oxoglutarate; Met180, Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the construction of the part of the active site binding 2-oxoglutarate; and Arg160 and Arg162 are important for binding an amino acid or peptide derived substrate.

- A method as claimed in any one of claims 21-23, wherein the said other enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.
- 25. A method as claimed in any one of claims 21-23, wherein the said other enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.
  - A method as claimed in any one of claims 21-23, wherein the said other enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.

